Unravelling Soft Components in the Shape Function for Inclusive B Decays

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Abstract

In the heavy-quark limit, the decay spectrum for radiative and semileptonic inclusive B-meson decays is determined by a universal structure function, i.e. the shape function. We study the constraints on the bilocal heavy-quark operator for the shape function from the QCD equations of motion and heavy-quark symmetry, and we obtain a new basis of nonlocal operators that reveals relevant soft components in the shape function. Those nonlocal operators represent the “kinetic energy distribution” of the $b$-quark inside the $B$-meson and the four-parton correlations with additional quarks and gluons. A corresponding local operator basis relevant for relating the shape function to HQET parameters is also given, and novel effects of the quark-gluon correlations are discussed.

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§1. Introduction

Inclusive $B$-meson decays, such as charmless semileptonic $B \to X_u \ell \bar{\nu}$ decays and penguin-induced $B \to X_s \gamma$ decays, are of special interest because they are sensitive probes of electroweak parameters as well as new physics. Theoretical analysis of the corresponding (differential) decay rates has been developed on the basis of the operator product expansion (OPE) as a power series in $\Lambda_{\text{QCD}}/m_b$.\textsuperscript{1} This provides justification for the parton model and also the power corrections to it in terms of matrix elements of local operators.\textsuperscript{2} It is known, however, that the usual OPE becomes singular near the kinematic endpoint $E/E_{\text{max}} \sim 1$ for the lepton (photon) energy spectrum in the decay $B \to X_u \ell \bar{\nu} (B \to X_s \gamma)$; the endpoint region plays an important role in experimental analysis, especially for the precise determination of the CKM matrix element $|V_{ub}|$ from $B \to X_u \ell \bar{\nu}$, avoiding large backgrounds from the decays into charmed particles, $B \to X_c \ell \bar{\nu}$. In the endpoint region, the hadronic decay products evolving from the $u$-quark ($s$-quark) in $B \to X_u \ell \bar{\nu} (B \to X_s \gamma)$ have large energy but small invariant mass, so that the hadronic final state becomes jet-like with collinear interactions of an outgoing light quark. This implies that the short-distance expansion is not applicable, receiving the light-cone singularity, and the OPE has to be reorganized with the resummation of the most singular terms.\textsuperscript{3)–4)} This is accomplished through the light-cone expansion, which is similar to the treatment in deep inelastic lepton-nucleon scattering (DIS). As the result, at the leading power of $\Lambda_{\text{QCD}}/m_b$, the shape of the decay spectrum is described by an analogue of the leading twist in the DIS, i.e., by the factorization formula, where a structure function corresponding to the nonperturbative, long-distance ($\sim 1/\Lambda_{\text{QCD}}$) contribution is convoluted with the perturbatively calculable function.\textsuperscript{3)–5)} The structure function, called the shape function, is process independent and universal in the sense that the same shape function determines the decay spectrum of both $B \to X_u \ell \bar{\nu}$ and $B \to X_s \gamma$. More rigorous treatments of the factorization with three relevant mass scales, hard ($m_b$), hard-collinear ($\sqrt{m_b \Lambda_{\text{QCD}}}$), and soft ($\Lambda_{\text{QCD}}$), have been presented recently in the framework of soft-collinear effective theory (SCET).\textsuperscript{6)–9)} Those treatments have shown that the perturbatively calculable function is composed of two parts, the hard function due to the hard corrections and the jet function due to hard-collinear fluctuations associated with the light-quark jet, and that the resulting factorization formulae for $B \to X_u \ell \bar{\nu}$ and $B \to X_s \gamma$ are valid to all orders in $\alpha_s$\textsuperscript{5)–8).}

One-loop corrections\textsuperscript{10)} as well as the resummation of large (leading and next-to-leading) endpoint logarithms\textsuperscript{5),7)–9),11)–13)} have been calculated for perturbatively calculable functions in the factorization formulae for $B \to X_u \ell \bar{\nu}$ and $B \to X_s \gamma$. Also for the shape function, one-loop renormalization group evolution has been studied by many authors.\textsuperscript{7)–9),13)–15)} Un-
Fortunately, however, our understanding of the nonperturbative boundary value in the corresponding evolution equation is still poor. There have been some attempts to constrain the boundary value of the shape function by estimating the relevant nonperturbative effects, e.g., trying to relate the moments of the shape function with the fundamental parameters in the heavy-quark effective theory (HQET),\(^3\),\(^4\),\(^16\),\(^17\) and examining the ambiguity ("infrared renormalons") of the perturbation series for the shape function.\(^5\),\(^13\) Guided by such constraints, one would construct ansätze for the shape function, and eventually fit them to experimental data to fix the remaining uncertainties.\(^18\),\(^19\)

In attempting to reach this goal, it is desirable to analyze the operator structure of the shape function in QCD and clarify the maximal model-independent constraints among the matrix elements of the relevant operators. However, a systematic study for this purpose has not yet been carried out. In this paper, we discuss a systematic operator analysis for the shape function. Our approach is based on the exact identity for the bilocal heavy-quark operator, which we derive from the QCD equations of motion and heavy-quark symmetry. Combined with the light-cone expansion of the bilocal operator to separate the longitudinal-momentum dependence from transverse one, it is possible to derive a differential equation that controls the longitudinal-momentum dependence of the shape function. We find that the corresponding differential equation involves the "source terms" given by matrix elements of a finite set of higher-dimensional nonlocal operators. Those nonlocal operators represent the "kinetic energy distribution" of the \(b\)-quark inside the \(B\)-meson and the four-parton correlations with additional quarks and gluons. Solving this differential equation, we express the shape function in terms of those nonlocal operators that explicitly represent the nonperturbative effects relevant for the shape function.

When deriving the differential equation from the exact operator identity, and also when solving the differential equation, we need to specify the boundary conditions for the shape function. In this paper, we employ the boundary conditions that the (non-negative) moments of the shape function as a function of the longitudinal momentum are finite. These conditions are equivalent to assuming that the nonlocal operators relevant to the shape function are the generating functions of the corresponding local operators via the Taylor expansion, and hold trivially when ignoring renormalization effects.\(^\ast\) However, recent results for the one-loop renormalization of the shape function in the \(\overline{\text{MS}}\) scheme claim that the renormalization effects completely modify the mathematical properties as well as the physical interpretation of the shape function. In particular, a "radiative tail" is generated for the momentum representation of the shape function, so that all non-negative moments become ultra-violet.

\(^\ast\) It is well known that similar conditions are satisfied by the structure functions in the DIS, and that they are preserved by including the radiative corrections.\(^23\)–\(^26\)
(UV) divergent.\(^7,8,13,14\) Because of this, the differential equation for the shape function and its solution discussed in this paper are exact up to the strong renormalization effects of order \(\alpha_s\). However, it is important to emphasize that actually our results are useful and indispensable beyond the lowest order in the perturbative effects, i.e., for obtaining the total behavior of the renormalized shape function: As noted in Refs. 7), 8), 13), the strong UV behavior in the renormalization effects implies that, for a consistent treatment and interpretation, the renormalized shape function should be further “factorized” into the “hard components” involving the radiative corrections and the “soft components” involving all the nonperturbative effects. In the matching calculation to perform this factorization, the first step is to list a basis of operators to describe the relevant soft components. The solution given in the present paper provides a basis of nonlocal operators as well as the corresponding local operator basis, including the four-parton correlation operators that were previously unknown. Furthermore, our solution provides the complete tree-level result for the hard components.

The remainder of this paper is organized as follows. In \(\S 2\) we demonstrate that the equations of motion and heavy-quark symmetry allow us to express the bilocal heavy-quark operator for the shape function in terms of a finite set of higher-dimensional nonlocal operators, which provides a new basis of nonlocal operators representing relevant soft components in the shape function. We also derive a corresponding local operator basis in \(\S 3\), which is relevant when relating the soft components of the shape function to the HQET parameters. In contrast to the previous works,\(^3,4,13,16,17\) our local operator basis is composed of an increasing number of operators with increasing dimension; in addition to a few first operators with low dimension, whose matrix elements give the well-known HQET parameters,\(^3,4,16\) we find “new” operators with higher dimensions, whose matrix elements provide the “generalized” HQET parameters that represent the “Fermi motion” of the \(b\)-quark as well as the four-parton correlation effects inside the \(B\)-meson. We also discuss simple estimates of some of these generalized HQET parameters and novel effects of the quark-gluon correlations. In \(\S 4\) we derive an explicit formula for the momentum representation of the shape function. Although this formula is subject to modification due to large radiative corrections, it deserves consideration, because it expresses the “Fermi motion” of the \(b\)-quark in an explicit analytic form and the four-parton correlation effects in an integral representation. In \(\S 5\) we present our conclusions.
§2. Nonlocal HQET operators and equations of motion

The factorization formulae for the decay spectrum in the inclusive $B$-meson decays are proved with the two-step matching, i.e., matching QCD onto SCET at a scale $\sim m_b$, followed by matching SCET onto HQET at a scale $\sim \sqrt{m_b A_{\text{QCD}}}$. The shape function is introduced at the second step by integrating out the final-state light-quark jet associated with the mass scale $\sqrt{m_b A_{\text{QCD}}}$, and it is defined as the $B$-meson matrix element of a gauge-invariant, bilocal light-cone operator in the HQET:

$$\langle \bar{B}(v)|\bar{h}_v(z)[z,0]|\bar{h}_v(0)|B(v)\rangle = \tilde{f}(t) = \int d\omega e^{i\omega t} f(\omega).$$  \hspace{2cm} (2.1)

Here $z^\mu$ denotes a light-like vector, $z^2 = 0$, $v^\mu$ is the 4-velocity of the $B$-meson ($v^2 = 1$), and $t = v \cdot z$. We choose the Lorentz frame of the system as $z^\mu = (0, z^-, 0_\perp)$ and $v^\mu = (v^+, v^-, 0_\perp)$, corresponding to the case in which the final-state jet momentum points in the “−” direction on the light-cone. $h_v(x)$ denotes the effective $b$-quark field, $b(x) \approx \exp(-im_b v \cdot x)h_v(x)$, and it is subject to the on-shell constraint $\not{v} h_v = h_v$. Here

$$[z,0] = P \exp\left(i g \int_0^1 d\xi z_\mu A^\mu(\xi z)\right)$$  \hspace{2cm} (2.2)

is the path-ordered gauge factor along the straight line connecting the points $z$ and $0$. For brevity, in the following, we do not show the path-ordered gauge factors connecting the constituent fields. We employ a mass-independent normalization of the $B$-meson state $|\bar{B}(v)\rangle$, such that $\langle \bar{B}(v)|\bar{B}(v')\rangle = v^0 (2\pi/m_B)^3 \delta^{(3)}(v - v')$, with $m_B$ the $B$-meson mass. The functions $\tilde{f}(t)$ and $f(\omega)$ give the coordinate and (residual) momentum representations of the shape function, respectively. Due to the heavy-quark spin symmetry, there appears no other independent function by taking matrix elements of the bilocal operators with other Dirac matrices inserted.

Actually, the shape function (2.1) depends on the scale $\mu$ at which the nonlocal light-cone operator is renormalized ($\sqrt{m_b A_{\text{QCD}}} \gtrsim \mu \gtrsim A_{\text{QCD}}$). It is known that the radiative corrections induce a Sudakov-type strong scale dependence on (2.1), governed by the corresponding cusp anomalous dimension,\(^5,13\)–\(^15\) and, corresponding to this effect, $\tilde{f}(t)$ in the $\overline{\text{MS}}$ scheme becomes singular for short distances: $\tilde{f}(0)$, as well as all derivatives of $\tilde{f}(t)$ at $t = 0$, diverge. As discussed in §1, however, such singular UV behavior can be factorized from the “soft components” of the shape function by an additional matching procedure, and we can ignore the renormalization in order to disentangle the operator structure relevant for the soft components. Therefore, in the following, we work with “naive” mathematical properties for (2.1) that are valid at lowest order in the perturbative effects, e.g., that $\tilde{f}(0) = 1$, and that $\tilde{f}(t)$
can be Taylor expanded about \( t = 0 \). With these boundary conditions, the physical meaning of \( f(\omega) \) is that it is the distribution of the residual momentum \( k^+ = \omega v^+ \) of the heavy quark inside the \( B \)-meson.\(^{a)\) A similar approach has been employed in Refs. 5) and 13) to analyze a few first local operators in the Taylor expansion of \( \bar{h}_v(z) h_v(0) \) about \( z_\mu = 0 \), considering the small \( t \) expansion of \( \tilde{f}(t) \). Our approach corresponds to an extension of the analysis given in Refs. 5) and 13) by treating the relevant nonlocal operator \( \bar{h}_v(z) h_v(0) \) directly. Although this is formally equivalent to treating all local operators in the Taylor expansion of \( \bar{h}_v(z) h_v(0) \) simultaneously, our nonlocal operator approach has the advantage of making the operator structure for the soft components of the shape function most transparent.

We can utilize the nonlocal operator technique, which has been developed for analyzing the (higher twist) nucleon structure functions\(^{23)-26)}\) (see also Refs. 28) and 29)\(^{b)\}). The nonperturbative dynamics of the \( b \)-quark, surrounded by the light quarks, antiquarks, and gluons, reveals itself as the response of the nonlocal operator \( \bar{h}_v(z) h_v(0) \) to the change of the interquark separation and/or total translation, but the total translation is irrelevant for the forward matrix elements. The relevant response of the nonlocal operator is described by the exact operator identity

\[
v^\mu \frac{\partial}{\partial x^\mu} \bar{h}_v(x) h_v(0) = \bar{h}_v(x) v \cdot \vec{D} h_v(0) + i \int_0^1 duu \bar{h}_v(x) gG_{\mu\nu}(ux)v^\mu x^\nu h_v(0) ,
\]

(2.3)

where \( x^\mu \) is not restricted on the light cone. \( \vec{D}_\mu = \vec{\partial}_\mu + igA_\mu \) and \( D_\mu = \partial_\mu - igA_\mu \) are the covariant derivatives, and \( G_{\mu\nu} = (i/g)[D_\mu, D_\nu] \) is the gluon field strength tensor. Taking the \( B \)-meson matrix element of the relation (2.3), the first term on the RHS vanishes, due to the HQET equations of motion \( \bar{h}_v v \cdot \vec{D} = 0 \). We take the light-cone limit, \( x_\mu \to z_\mu \); for the calculation of the LHS, we actually need to extend the definition (2.1) to the case in which the interquark separation is not light-like, where we have

\[
\langle \bar{B}(v) | \bar{h}_v(x) h_v(0) | \bar{B}(v) \rangle = \tilde{f}(v \cdot x) + x^2 \tilde{F}(v \cdot x) + \mathcal{O}(x^4) ,
\]

(2.4)

while, for the second term on the RHS, we introduce a three-parton correlation function \( \tilde{R}(t, u) \) as

\[
\langle \bar{B}(v) | \bar{h}_v(x) gG_{\mu\nu}(ux) x^\nu h_v(0) | \bar{B}(v) \rangle = \frac{1}{2} \left( x_\mu - \frac{x^2}{v \cdot x} v_\mu \right) \left[ \tilde{R}(t, u) + \mathcal{O}(x^2) \right] .
\]

(2.5)

Then we obtain the following constraint equation due to the equations of motion:

\[
\frac{d\tilde{f}(t)}{dt} + 2t\tilde{F}(t) = \frac{i}{2} t \int_0^1 duu \tilde{R}(t, u) .
\]

(2.6)

\(^a)\) Actually, the validity of this “probabilistic interpretation” appears to be critical, due to nonperturbative as well as perturbative effects. (See the discussion in §§4 and 5 below.)

\(^b)\) A similar extension has been employed for the \( B \)-meson light-cone wavefunctions.\(^{27)}\)
This equation is formally similar to the corresponding differential equations for the twist-3 nucleon structure functions, but an important difference is the participation of $\tilde{F}(t)$ in (2.6), which expresses the effect due to the deviation from the light-cone, as in (2.4). For the nucleon case, contributions of this type correspond to twist-4 effects and decouple from the equations at the twist-3 level, because the twist defined as “dimension minus spin” of the relevant operators is a good quantum number. Although the twist counting of the shape function (2.1) would be twist-3, such a “conventional” twist is no longer a useful concept in the HQET.

It is straightforward to see that the insertion of an arbitrary Dirac matrix $\Gamma$ into (2.3)-(2.4) does not lead to a new equation for $\tilde{f}(t)$. This is unlike the case for the $B$-meson wavefunctions, and it is due to so strong constraints on the forward matrix elements imposed by the heavy-quark spin symmetry.

To proceed, we analyze the explicit operator structure of $\tilde{F}(t)$ in (2.6), which can be extracted from the next-to-leading term in the light-cone expansion of the nonlocal operator $\tilde{h}_v(x)h_v(0)$ [see (2.4)]. For this purpose, we utilize an elegant method to construct the light-cone expansion: The leading term (lt) in the light-cone expansion, corresponding to the leading twist operator in the DIS, obeys the equation

$$\frac{\partial^2}{\partial x_\mu \partial x^\mu} [\tilde{h}_v(x)h_v(0)]_{lt} = 0 , \quad (2.7)$$

which ensures that all local operators arising in the Taylor expansion are traceless. A formal solution is

$$[\tilde{h}_v(x)h_v(0)]_{lt} = \tilde{h}_v(x)h_v(0)$$

$$+ \sum_{n=1}^{\infty} \left( \frac{-x^2}{4} \right)^n \frac{1}{n!} \int_0^1 \frac{du}{u^n} \left( \frac{\partial^2}{\partial x_\mu \partial x^\mu} \right)^n \tilde{h}_v(ux)h_v(0) . \quad (2.8)$$

To order $x^2$, we obtain

$$\tilde{h}_v(x)h_v(0) = [\tilde{h}_v(x)h_v(0)]_{lt} + \frac{x^2}{4} \int_0^1 \frac{du}{u} \frac{\partial^2}{\partial x_\mu \partial x^\mu} \tilde{h}_v(ux)h_v(0) + \mathcal{O}(x^4) . \quad (2.9)$$

Actually, the first term on the RHS of (2.4) contains the $\mathcal{O}(x^2)$ term as well as the leading term. To separate contributions of different powers in $x^2$, it is convenient to exploit the light-cone expansion of $\exp(i\omega v \cdot x)$ entering into the definition of the momentum representation of $\tilde{f}(v \cdot x)$, (24), (29)

$$e^{i\omega v \cdot x} = [e^{i\omega v \cdot x}]_{lt} - \frac{\omega^2 x^2}{4} \int_0^1 du u e^{i\omega v \cdot x} + \mathcal{O}(x^4) , \quad (2.10)$$
where \([e^{iωv·x}]_t\) is defined by a straightforward generalization of the procedure \([\ldots]_t\) of (2.8) to an arbitrary function of \(x\). Substituting (2.9)-(2.10) into (2.4) and comparing both sides of the resulting equation, the leading terms reproduce the definition (2.1), and we get, from the next-to-leading \(O(x^2)\) terms,

\[
\tilde{F}(t) = \frac{1}{4} \int_0^1 du u \tilde{Φ}(ut) + \frac{1}{4} \int dω ω^2 f(ω) \int_0^1 du ue^{iωt},
\]

with

\[
\tilde{Φ}(t) = \langle \tilde{B}(v)|\frac{∂^2}{∂x_μ∂x_ν} \tilde{h}_v(x)h_v(0)|\tilde{B}(v)\rangle \bigg|_{x→z}. \tag{2.12}
\]

Here, the second term on the RHS of (2.11) is the analogue of Nachtmann’s correction in the DIS. An important point is that this term depends on \(f(ω)\), and it produces an additional term involving \(\tilde{f}(t)\) in (2.6). Substituting (2.11) into (2.6), we obtain

\[
t \frac{d\tilde{f}(t)}{dt} + \tilde{f}(t) - 1 = t^2 \int_0^1 du u \left(i \tilde{R}(t, u) - \tilde{Φ}(ut)\right). \tag{2.13}
\]

Here the RHS involves \(\tilde{Φ}\) of (2.12), which is concerned with the effects of the transverse as well as longitudinal motion of the \(b\)-quark inside the \(B\)-mesons. To reveal its physical content further, the following exact identity is useful:

\[
\frac{∂^2}{∂x_μ∂x_ν} \tilde{h}_v(x)h_v(0) = \tilde{h}_v(x) (\tilde{D}_μ)^2 h_v(0) + 2i \int_0^1 du u \frac{∂}{∂x_μ} \tilde{h}_v(x) gG_{μν}(ux) x'ν h_v(0)
\]

\[
- i \int_0^1 du u^2 \tilde{h}_v(x) [D_μ, gG_{μν}(ux)] x'ν h_v(0)
\]

\[
+ 2 \int_0^1 du u \int_0^ux'ν \tilde{h}_v(x) gG_{μν}(ux) x'ν gG_{μρ}(sx) x_ρ h_v(0). \tag{2.14}
\]

This can be derived straightforwardly by a method similar to (2.3). Substituting (2.14) into (2.12), the replacement \(\tilde{D}_μ → \tilde{D}_μ → D_μ \equiv D_μ - v_μ v · D\) can be made in the first term on the RHS by using the equations of motion for the effective heavy-quark field. Similarly, the equations of motion for the gluons imply \([D_μ, G_{μν}] = -gt^a \sum (v_ν \tilde{h}_v t^a h_v + \bar{q}t^a γ_ν q)\), with the summation \((\sum)\) over the heavy \((h_v)\) and light \((q)\) flavors. Therefore, (2.12) can be expressed in terms of a set of many-body nonlocal operators. This pattern is similar to that for the twist-4 effects in the DIS\(^{23,24}\) but one important difference is that the covariant derivative for the transverse direction, \(D_μ\), acting on the quark fields cannot be completely eliminated in the present case; participation of such a transverse derivative in a complete set of the higher-dimensional operators is typical of the HQET\(^{20,21}\). In fact, the corresponding operator in

\(^*\) A similar identity for the case of the light quarks is discussed in Ref. 29.)
(2.14) plays an important role in describing the Fermi motion effects in the $B$-mesons, as we show below.

The matrix element of the derivative of the three-body operator in (2.14) can be calculated using (2.5). An important observation is that this contribution cancels the first term $i \tilde{R}(t, u)$ on the RHS of (2.13), so that the three-parton correlation $\tilde{R}$ decouples from our differential equation. For the remaining terms, we define

$$
\langle \bar{B}(v) | \bar{h}_v(z) (D_{\perp \mu})^2 h_v(0) | \bar{B}(v) \rangle = \tilde{K}(t),
$$

(2.15)

$$
\langle \bar{B}(v) | \bar{h}_v(z) [D^\mu, g G_{\mu\nu}(uz)] z^\nu h_v(0) | \bar{B}(v) \rangle = \tilde{W}(t, u),
$$

(2.16)

$$
\langle \bar{B}(v) | \bar{h}_v(z) g G_{\mu\nu}(uz) z^\nu g G^{\mu\rho}(sz)_z z^\rho h_v(0) | \bar{B}(v) \rangle = t^2 \tilde{Y}(t, u, s).
$$

(2.17)

Here, $\tilde{K}(t)$ can be interpreted as the “kinetic energy distribution” of the $b$-quark inside the $B$-meson, while $\tilde{W}(t, u)$ and $\tilde{Y}(t, u, s)$ are the four-parton correlations with additional quarks and gluons, respectively. We denote the RHS of (2.13) as $\tilde{J}(t)$ and substitute (2.15)-(2.17) into it. We then obtain

$$
\tilde{J}(t) = \int_0^t dt' \left\{ -t' \tilde{K}(t') + it'^2 \int_0^1 du u^2 \tilde{W}(t', u) - 2t'^3 \int_0^1 du \int_0^u ds ss \tilde{Y}(t', u, s) \right\}.
$$

(2.18)

Regarding $\tilde{J}(t)$ as the “source” term, (2.13) is immediately integrated to give, with the condition $\tilde{f}(0) = 1$,

$$
\tilde{f}(t) = 1 + \frac{1}{t} \int_0^t d\tau \tilde{J}(\tau).
$$

(2.19)

Thus $\tilde{f}(t)$ is completely re-expressed in terms of a set of nonperturbative functions, $\tilde{K}(t)$, $\tilde{W}(t, u)$ and $\tilde{Y}(t, u, s)$, corresponding to the higher-dimensional nonlocal operators.

§3. Local operator basis and HQET parameters

In this section we derive a basis of local composite operators to represent the soft components of the shape function, and we discuss the HQET parameters as matrix elements of these operators. It is straightforward to expand the solution (2.19) in a power series in $t$ as

$$
\tilde{f}(t) = 1 + \sum_{n=1}^{\infty} \frac{(it)^n}{n!} A_n,
$$

(3.1)

where the $n$-th term gives the nonperturbative power corrections of order $(\Lambda_{QCD} t)^n$. We obtain

$$
A_n = \frac{n-1}{n+1} \kappa_{n-2} - \frac{1}{n(n+1)} \left[ \sum_{k=0}^{\frac{n+1}{2}} \frac{1}{(k+1)(k+2)} \right.
$$

9
which are generated from the Taylor expansion of (2.15)-(2.17) about $z_\mu = 0$.

Also, (3.8) as well as (3.6) coincides with the corresponding results discussed in the earlier works [see also (2.16)]. Equation (3.6) coincides with that obtained in Refs. 5) and 13).

Note that $K_n$, $W_{l,k}$ and $Y_{l,k}^m$ denote matrix elements of the local operators, which are generated from the Taylor expansion of (2.15)-(2.17) about $z_\mu = 0$:

\[
\begin{align*}
K_n &= \frac{1}{(v^+)n} \langle \bar{B}(v)|h_v^*(iD^+)^n(D_{\perp \mu})^2 h_v|\bar{B}(v) \rangle , \\
W_{l,k} &= -\frac{1}{(v^+)l+l+1} \sum_q \langle \bar{B}(v)|h_v^*(iD^+)^k g^2 t^a q t^a \gamma^+ q(iD^+)^l h_v|\bar{B}(v) \rangle , \\
Y_{l,k}^m &= \frac{1}{(v^+)l+l+m+2} \langle \bar{B}(v)|h_v^*(iD^+)^k g G^\mu + (iD^+)^m g G^{\mu +}(iD^+)^l h_v|\bar{B}(v) \rangle .
\end{align*}
\]

Note that $W_{l,k}$ and $Y_{l,k}^m$ are symmetric under the interchange $l \leftrightarrow k$, which follows from the behavior of the corresponding matrix elements (3.4) and (3.5) under the parity transformation combined with the time-reversal transformation. Equation (3.2) gives, for $n = 1$ and 2,

\[
A_1 = 0, \quad A_2 = \frac{1}{3} K_0 = -\frac{\lambda_1}{3} ,
\]

with the fundamental HQET parameter $\lambda_1$ related to the average kinetic energy of the heavy quark inside the $B$-mesons,\(^{20,21}\)

\[
\lambda_1 = \langle \bar{B}(v)|h_v^*(iD_{\perp \mu})^2 h_v|\bar{B}(v) \rangle ,
\]

and, for $n = 3$,

\[
A_3 = -\frac{1}{6} W_{0,0} = \frac{1}{6} \sum_q \langle \bar{B}(v)|h_v g^2 t^a q t^a \gamma^+ q h_v|\bar{B}(v) \rangle ,
\]

where the four-quark operator is related to the quark-gluon Darwin operator by the equations of motion [see also (2.16)]. Equation (3.7) coincides with that obtained in Refs. 5) and 13). Also, (3.8) as well as (3.6) coincides with the corresponding results discussed in the earlier works.\(^{3,4,16}\)

We note that those works analyzed the constraints resulting from the equations of motion on the matrix elements of the corresponding local operator,

\[
A_n = \frac{1}{(v^+)^n} \langle \bar{B}(v)|h_v^*(iD^+)^n h_v|\bar{B}(v) \rangle ,
\]

which follows from (2.1).
Furthermore, (3.2) gives new results for \( n \geq 4 \),

\[
A_4 = \frac{3}{5} K_2 - \frac{2}{5} W_{0,1} - \frac{3}{10} \mathcal{Y}_{0,0}^0 ,
\]

\[
A_5 = \frac{2}{3} K_3 - \frac{7}{15} W_{0,2} - \frac{1}{5} W_{1,1} - \frac{4}{15} \mathcal{Y}_{0,0}^1 - \frac{11}{15} \mathcal{Y}_{0,1}^0 ,
\]

and so forth. Therefore, the operators in (3.3)-(3.5), whose matrix elements give

\[
A_{n-2}, \quad \mathcal{W}_{k,n-k} \quad (k = 0, 1, 2, \cdots, \left\lfloor \frac{n-3}{2} \right\rfloor) ,
\]

\[
\mathcal{Y}_{l,k-l}^{n-k-l} \quad (k = 0, 1, 2, \cdots, n-4; \quad l = 0, 1, 2, \cdots, \left\lfloor \frac{k}{2} \right\rfloor) ,
\]

form a basis of local operators of dimension \( n + 3 \) and contribute to \( A_n \). This implies that for \( n \gg 1 \) there are \( \sim n^2/4 \) independent local operators participating in \( A_n \).

Here it is worth studying the details of the new nonperturbative matrix elements contributing to \( A_4 \), because these matrix elements provide a generalization of the HQET parameters. \( K_2 \) and \( W_{0,1} \), given by (3.3) and (3.4), can be related to the “trace part” of the corresponding operators as

\[
K_2 = \frac{1}{3} \langle \bar{B}(v) | \bar{h}_v (\langle D_{\perp \mu} \rangle^2)^2 h_v | \bar{B}(v) \rangle ,
\]

\[
W_{0,1} = \frac{i}{3} \sum_q \langle \bar{B}(v) | \bar{h}_v g^2 \bar{q} t^a \gamma_\mu q D_{\perp \mu} h_v | \bar{B}(v) \rangle .
\]

Thus \( K_2 > 0 \), and a comparison of (3.13) with (3.7) leads to the rough estimate \( K_2 \sim \lambda^2 \).

The matrix element (3.14) involving the four-quark operator can be evaluated in the vacuum saturation (“factorization”) approximation\(^\ast\) as

\[
W_{0,1} \approx -\pi \frac{N_c^2 - 1}{6N_c^2} \alpha_s f_B^2 m_B \bar{\Lambda} ,
\]

with the usual decay constant \( f_B \), defined as \( \langle 0 | \bar{q} \gamma^\mu \gamma_5 h_v | B(v) \rangle = i f_B \sqrt{m_B/2} v^\mu \). Here \( \bar{\Lambda} \) represents the asymptotic value of the mass difference \( m_B - m_b \) between the \( B \)-meson and the \( b \)-quark,\(^{20,21}\) and it can be identified with the effective mass of the light degrees of freedom in the \( B \)-meson. Using phenomenological values for the parameters on the RHS of (3.15) leads to \( W_{0,1} \sim -\lambda^2 \). Contrastingly, \( \mathcal{Y}_{0,0}^0 \) of (3.5) cannot be estimated in a simple manner, but in the \( B \)-meson rest frame it is expressed in terms of the chromoelectric and chromomagnetic fields as

\[
\mathcal{Y}_{0,0}^0 = -\frac{2}{3} \langle \bar{B}(v = 0) | \bar{h}_v g^2 (E^2 + B^2) | \bar{B}(v = 0) \rangle ,
\]

\(^\ast\) This approximation gives the estimate \( W_{0,0} \approx \pi [(N_c^2 - 1)/2N_c^2] \alpha_s f_B^2 m_B \) of (3.16).
so that $\mathcal{V}_{0,0}^0 < 0$. Here we note that a comparison between (3.6) and (3.9) with $n = 4$ suggests the rough estimate $A_4 \sim \lambda_1^2$, and combined with the relation (3.10), we would expect $\mathcal{V}_{0,0}^0 \sim -\lambda_1^2$. In principle, $A_5$ of (3.11) could be analyzed similarly, but it involves the five new nonperturbative matrix elements and is much more complicated.

When $A_{QCD}t$ is not so small compared to 1, which is the case in the endpoint region for the lepton (photon) energy spectrum in $B \to X_u \ell \bar{\nu}$ ($B \to X_s \gamma$), the higher-order power corrections ($A_{QCD}t)^n$ are important to determine the behavior of $\hat{f}(t)$. Among the parameters (3.8)-(3.11) involved in $A_n$, the experimental value is known for $K_0 (= -\lambda_1)$ of (3.6) only.\(^8,31\) Hopefully, further information regarding these generalized HQET parameters will be obtained from nonperturbative calculations with, e.g., lattice QCD\(^\ast\ast\) and QCD sum rules.

§4. Fermi motion and four-parton correlation effects

In this section we derive an explicit formula for the momentum representation of the shape function, which is exact up to perturbative $\mathcal{O}(\alpha_s)$ corrections. Although this formula suffers from (large) perturbative corrections, it is useful for obtaining some insight into the relevant nonperturbative effects, the Fermi motion of the $b$-quark, and the four-parton correlation effects, without recourse to the $t$-expansion as in (3.1). For this purpose, we derive the Fourier transformation of (2.19) into the residual momentum representation [see (2.1)]. We obtain $f(\omega) = \delta(\omega) + [\text{contribution from } \tilde{J}]$. Clearly, the first term, $\delta(\omega)$, reflects the lack of heavy-quark motion inside the $B$-mesons in the “non-interacting limit”, and the above decomposition of $f(\omega)$ into the “free” term $\delta(\omega)$ and the “interaction-dependent” contribution from $\tilde{J}$ would be unsuitable to treat the nonperturbative part in the shape function. In order to avoid such an “artificial” singularity, we rearrange the terms in (2.19). Actually, it is more convenient to make the corresponding rearrangement in our differential equation (2.13) by moving a certain term from the “source” on the RHS to the LHS, and then solve the resulting equation with the new source. We decompose $\tilde{K}(t)$ in (2.18) as [see (2.15)]

$$\tilde{K}(t) = \sigma^2 \hat{f}(t) + \delta \tilde{K}(t) , \quad (4.1)$$

\(^\ast\) The identity between matrix elements of the local operators, which is implied by (3.9) with $n = 4$ and (3.10), would be subject to the perturbative $\mathcal{O}(\alpha_s)$ corrections, but these corrections do not affect this simple estimate.

\(^\ast\ast\) For the regions with $m_b \gg 1/t$, these power corrections are enhanced compared with the usual subleading corrections, which are suppressed by powers of $A_{QCD}/m_b$.\(^32\) Physically, this corresponds to the situation in which the decay spectra in the endpoint region is smeared over a range $\Delta$ with $m_b \gg \Delta \gg A_{QCD}$.\(^7,9\)

\(^\ast\ast\ast\) For recent progress in treating matrix elements of $B$-mesons in lattice QCD, see, e.g., Ref. 33).
and move the first term with the constant $\sigma^2$ to the LHS of (2.13). The residual term $\delta \tilde{K}(t)$ is treated as a source term. The explicit form of the residual term reads
\[
\delta \tilde{K}(t) = \langle \bar{B}(v)|\bar{h}_v(z)\left((\tilde{D}_{\pm \mu})^2 - \sigma^2\right)h_v(0)|\bar{B}(v)\rangle .
\] (4.2)

The rearrangement using (4.1) is motivated by the observation that the first term is special among the terms on the RHS of (2.18): Among the nonlocal operators of (2.15)-(2.17) contributing to (2.18), the operator for $\tilde{K}(t)$ has the lowest mass dimension, and it is expected to play a dominant role. In fact, only this contribution is of a bilocal nature as (2.15), as in the case of the shape-function operator (2.1), while the other contributions come from genuine many-body operators. Noting the properties of the higher twist nucleon structure functions in the DIS,\textsuperscript{30} we conjecture that multi-parton correlation effects with increasing numbers of partons are less important. We note that the operator for $\tilde{K}(t)$ is a nonlocal version of the kinetic energy operator of (3.7), and it should be relevant to the Fermi motion of the $b$-quark inside the $B$-meson; in (4.1) we have extracted the part proportional to $\tilde{f}(t)$ from $\tilde{K}(t)$ on the basis of the fact that $\tilde{K}(t)$ and $\tilde{f}(t)$ have similar bilocal natures, and thus $\sigma$ would eventually correspond to the “average measure” of the transverse quark motion, as $\sigma^2 \sim -\lambda_1$ [note that $\tilde{K}(0) = -\lambda_1$]. However, for the time being, we can leave $\sigma$ as an arbitrary parameter.

In momentum space, our differential equation now reads
\[
(\omega^2 - \sigma^2) \frac{df(\omega)}{d\omega} = -I(\omega) .
\] (4.3)

Here, the source $I(\omega)$, defined as $d\tilde{J}(t)/dt\big|_{\tilde{K} \to \delta \tilde{K}} \equiv i \int d\omega e^{i\omega t} I(\omega)$, is given explicitly as [see (2.18)]
\[
I(\omega) = -\frac{d}{d\omega} \delta K(\omega) + \int_{-\infty}^{\omega} d\alpha P \int_{-\infty}^{\infty} d\beta \frac{1}{\alpha - \beta} \left( \frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial \beta^2} \right) W(\alpha, \beta)
\]
\[
+ 2 \int_{-\infty}^{\omega} d\alpha P \int_{-\infty}^{\infty} d\beta \int_{-\infty}^{\infty} d\xi \frac{1}{\alpha - \beta} \left\{ \left[ \frac{1}{\alpha - \xi} \left( \frac{\partial}{\partial \alpha} + \frac{\partial}{\partial \xi} \right) \right]^2 \right.
\]
\[
+ \frac{1}{\beta - \xi} \left( \frac{\partial}{\partial \beta} + \frac{\partial}{\partial \xi} \right)^2 + \frac{1}{(\alpha - \xi)^2} \left( \frac{\partial}{\partial \alpha} + \frac{\partial}{\partial \xi} \right)^2
\]
\[
+ \frac{1}{(\alpha - \xi)(\beta - \xi)} \left[ \frac{\partial}{\partial \beta} + \frac{\partial}{\partial \xi} \right] Y(\alpha, \beta, \xi) - \frac{1}{\xi^2} \frac{\partial}{\partial \alpha} Y(\alpha - \xi, \beta, \alpha) \right\} ,
\] (4.4)

where “P” denotes the principal value, and we have introduced the momentum representation for the relevant matrix elements (4.2), (2.16), and (2.17) as
\[
\delta \tilde{K}(t) = \int d\omega \ e^{i\omega t} \delta K(\omega) ,
\] (4.5)
\[
\bar{W}(t, u) = \int d\omega \, d\omega' e^{i\omega't - i(\omega' - \omega)ut} W(\omega, \omega'), \quad (4.6)
\]
\[
\bar{Y}(t, u, s) = \int d\omega d\omega' d\xi \, e^{i\omega't - i(\omega' - \xi)ut - i(\xi - \omega)s} Y(\omega, \omega', \xi). \quad (4.7)
\]

We note that the parity transformation combined with the time-reversal transformation implies the symmetry properties

\[
W(\omega, \omega') = W(\omega', \omega), \quad Y(\omega, \omega', \xi) = Y(\omega', \omega, \xi), \quad (4.8)
\]

and hermiticity guarantees that \(W(\omega, \omega')\) and \(Y(\omega, \omega', \xi)\) are real functions. For both functions, the variable \(\omega\) has the physical meaning of the residual light-cone momentum carried by the \(b\)-quark. The quantity \(\omega' - \omega\) for \(W(\omega, \omega')\) represents the light-cone momentum carried by the gluon or the light \(q\bar{q}\)-pair, while \(\xi - \omega\) and \(\omega' - \xi\) for \(Y(\omega, \omega', \xi)\) represent the light-cone momenta carried by the gluons. By inserting a complete set of states between the constituent fields, we also get the support property: \(W(\omega, \omega')\), as well as \(Y(\omega, \omega', \xi)\), vanishes unless \(\omega < \bar{\Lambda}\) and \(\omega' < \bar{\Lambda}\). Similarly, we deduce that \(\delta K(\omega)\) is a real function that vanishes unless \(\omega < \bar{\Lambda}\). Using these symmetry and support properties of \(\delta K, W\) and \(Y\), it is straightforward to see that \(I(\omega)\) of (4.4) vanishes unless \(\omega < \bar{\Lambda}\).

We solve (4.3) with the boundary conditions \(f(\omega) = 0\) for \(\omega \to \pm \infty\) and the normalization condition \(\int d\omega f(\omega) = \tilde{f}(0) = 1\) in the form

\[
f(\omega) = f^{(0)}(\omega) + f^{(1)}(\omega), \quad (4.9)
\]

where \(f^{(0)}(\omega)\) is the solution with the source \(I(\omega)\) set to zero, while \(f^{(1)}(\omega)\) denotes the piece induced by \(I(\omega)\). It is straightforward to obtain the analytic solution

\[
f^{(0)}(\omega) = \frac{1}{2\sigma} \left\{ \theta(\omega + \sigma) - \theta(\omega - \sigma) \right\}, \quad (4.10)
\]

which satisfies \(\int d\omega f^{(0)}(\omega) = 1\). Also, the solution for \(f^{(1)}(\omega)\) reads

\[
f^{(1)}(\omega) = \frac{1}{2\sigma} \left( \int_{-\infty}^{\infty} d\omega' \frac{I(\omega')}{\omega' - \sigma} - \int_{-\infty}^{\infty} d\omega' \frac{I(\omega')}{\omega' + \sigma} \right), \quad (4.11)
\]

which satisfies \(\int d\omega f^{(1)}(\omega) = 0\). The solution (4.9) with (4.10) and (4.11) represents an explicit formula for the shape function, which satisfies the HQET equations of motion exactly.

We note that, if we take the limit \(\sigma \to 0\), we get \(f^{(0)}(\omega) \to \delta(\omega)\), so that (4.10) and (4.11) would reduce to the “singular” decomposition of \(f(\omega)\) without the rearrangement using (4.1). Therefore, (4.9) involves a nonperturbative effect represented by the parameter \(\sigma\), which smears the singular behavior of \(\delta(\omega)\). If we choose, e.g., \(\sigma = \sqrt{-\lambda_1}\), the corresponding effect
would be interpreted as the Fermi motion effect of the $b$-quark inside the $B$-meson. This choice can be useful in practice, because, in the coordinate representation, we have

$$f^{(0)}(t)\big|_{\sigma=\sqrt{-\lambda_1}} = \frac{\sin \left(\sqrt{-\lambda_1} t\right)}{\sqrt{-\lambda_1} t} = 1 + \sum_{k=1}^{\infty} \frac{t^{2k} \lambda_1^k}{(2k)! (2k+1)},$$  \hspace{1cm} (4.12)$$

and the expansion on the RHS reproduces the first three terms of (3.1) exactly [see (3.6), and note that $f^{(1)}(t)\big|_{\sigma=\sqrt{-\lambda_1}} = it^3 W_{0,0}/36 + O(t^4)]$. In fact, “flat distribution” (4.10) with $\sigma = \sqrt{-\lambda_1}$ exhibits behavior consistent with the Gaussian distribution around $\omega = 0$ with the width $\sqrt{-\lambda_1}$, which was proposed in Refs. 5) and 13) as a nonperturbative ansatz valid in the vicinity of $\omega = 0$. As an alternative to the choice $\sigma = \sqrt{-\lambda_1}$, one may employ another “optimized” choice for $\sigma$, which makes $\delta \tilde{K}(t)$ of (4.2) “small”, so that $\delta \tilde{K}(t)$ could be treated as a perturbation.

It is well known that (2.1) should obey $f(\omega) = 0$ for $\omega > \bar{\Lambda}$.3),4),16) Using the above-mentioned support property for $I(\omega)$, it is straightforward to show that our solution (4.9) indeed vanishes unless $\omega < \bar{\Lambda}$, reproducing the correct support property.

Our solution reveals that the shape function is subject to nonperturbative effects due to the multi-parton correlation with additional quarks and gluons, which are represented by $W(\omega, \omega')$ and $Y(\omega, \omega', \xi)$, as in (4.11), (4.4). This indicates that $f(\omega)$ is actually a complicated multi-particle object beyond a “simple” momentum distribution function. This is in contrast to the leading-twist nucleon structure functions in the DIS, but it is reminiscent of the character of the higher-twist ones.23),25),26) Our results, (4.11) and (4.4), are exact to lowest order in the perturbative effects, but the multi-particle character of $f(\omega)$ should persist when perturbative corrections are included.

§5. Conclusion

The shape function of the $B$-meson is an important ingredient in the factorization formula of the differential rates of inclusive $B$-meson decays, such as $B \to X_\gamma \gamma$ and $B \to X_u l \bar{\nu}$. We studied the “soft components” of the shape function separately from the “hard (perturbative) components” relevant to its scale dependence, and we studied the model-independent constraints on the soft components in the heavy quark limit. From the equations of motion and heavy-quark symmetry constraints, we derived a differential equation that relates the longitudinal-momentum dependence of the shape function to matrix elements of the novel nonlocal operators. Solving this equation, we obtained a new basis of nonlocal operators, which describes the relevant soft components of the shape function in terms of the kinetic

\footnote{This is actually satisfied even in the case $\sigma > \bar{\Lambda}$, as well as for $\sigma \leq \bar{\Lambda}$.}
energy distribution and the four-parton correlations. We also derived the relations among the matrix elements of local operators with arbitrary numbers of covariant derivatives. These relations not only reproduce all the known results for a few covariant derivatives but also include new relations for more covariant derivatives. These relations are exact only when we ignore the perturbative effects, but they are useful beyond the lowest order in the perturbative effects for the purpose of finding a basis of independent local operators with the same dimension. Our relations indicate that the local operator basis is composed of an increasing number of operators with increasing dimensions whose matrix elements give the generalized HQET parameters that represent the Fermi motion of the $b$-quark as well as the four-parton correlation effects inside the $B$-meson. Our differential equation also yields the momentum representation $f(\omega)$ as a sum of the part $f^{(0)}(\omega)$ involving the Fermi motion and the additional part $f^{(1)}(\omega)$ induced by more sophisticated correlation effects. The behavior of the “leading” part, $f^{(0)}(\omega)$, appears to be consistent with the existing nonperturbative ansatz\(5,13\) for the shape function. Our momentum-representation formula is again exact up to perturbative corrections, but it provides insight into model building of the relevant nonperturbative effects.

Our results reveal that, due to nonperturbative effects, $f(\omega)$ is a much more complicated object than the simple momentum distribution of the $b$-quark inside the $B$-meson: Nonperturbative effects induce the mixing of additional dynamical quarks and gluons, so that the shape function contains the soft components that represent the multi-particle correlation effects. In connection to this, it is interesting to note that a probabilistic interpretation of $f(\omega)$ as the momentum distribution has been questioned from a different point of view, noting that $\int d\omega f(\omega)$ is negatively divergent, due to the perturbative effects in §1.7, 8.

The “full” shape function $f(\omega)$ entering into the factorization formula for the inclusive decay rates is obtained by combining the soft components with the hard components through the matching procedure. We emphasize that $(3.12)$ with $(3.3)-(3.5)$ provides a local operator basis that is necessary for parameterizing the soft components in the matching calculation. Furthermore, $(3.11)$ with $(3.2)$ completes the matching at the tree level for operators of arbitrary dimension, and the corresponding leading-order matching coefficients can be easily read off from this formula. One can proceed to the one-loop matching calculations using our operator basis, and the loop effects will produce the mixing coefficients at the next-to-leading order between the operators with the same dimension. Also, the nonlocal operator basis provided by $(2.15)-(2.17)$ may be useful, and $(2.19)$ with $(3.10)$ and $(4.11)$ completes the corresponding leading-order matching in the coordinate (momentum) space. Using the results of the matching calculations, a detailed study of the interplay between...
the strong perturbative effects in the hard components, which generate a Sudakov-type scale dependence, and the nonperturbative effects in the soft components, which have been unraveled in this paper, should clarify the behavior of the full shape function and its roles in decay rates. This will be studied in a separate publication.

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