Published for SISSA by Springer

Received: *September 16, 2022*
Revised: *November 11, 2022*
Accepted: *November 11, 2022*
Published: *November 17, 2022*

Resolving charged hadrons in QED — gauge invariant interpolating operators

Saad Nabeebaccus[a] **and Roman Zwicky**[b]

[a] *Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France*
[b] *Higgs Centre for Theoretical Physics, School of Physics and Astronomy, University of Edinburgh, Edinburgh EH9 3JZ, Scotland, U.K.*

E-mail: saad.nabeebaccus@ijclab.in2p3.fr, roman.zwicky@ed.ac.uk

Abstract: Standard interpolating operators for charged mesons, e.g. $J_B = \bar{b} i\gamma_5 u$ for B^-, are not gauge invariant in QED and therefore problematic for perturbative methods. We propose a gauge invariant interpolating operator by adding an auxiliary charged scalar Φ_B, $\mathcal{J}_B^{(0)} = J_B \, \Phi_B$, which reproduces all the universal soft and collinear logs. The modified LSZ-factor is shown to be infrared finite which is a necessary condition for validating the approach. At $\mathcal{O}(\alpha)$, this is equivalent to a specific Dirac dressing of charged operators. A generalisation thereof, using iterated integrals, establishes the equivalence to all orders and provides a transparent alternative viewpoint. The method is discussed by the example of the leptonic decay $B^- \to \ell^- \bar{\nu}$ for which a numerical study is to follow. The formalism itself is valid for any spin, flavour and set of final states (e.g. $B^- \to \pi^0 \ell^- \bar{\nu}$).

Keywords: Precision QED, Bottom Quarks

ArXiv ePrint: 2209.06925

https://doi.org/10.1007/JHEP11(2022)101

JHEP11(2022)101

Contents

1 Introduction

Scalar QED or the point-like approximation is a consistent framework which works numerically well in many cases, but precision in CKM matrix elements and testing of lepton flavour universality [1, 2] are calling for stucture-dependent computations.[1] Approaches include chiral perturbation theory (ChPT) [5–7], soft collinear effective theory (SCET) [8, 9] and lattice Monte Carlo simulations (with a range of methods to contain the massless photon in finite volume [10–13] and applications thereof in [14–18]). ChPT applies to low energy physics and might be viewed as a successful expansion around the point-like approximation where the challenge relies in determining the finite counterterms. In SCET, mesons are described by light-cone distribution amplitudes which necessitate the introduction of

[1] Scalar QED is sufficient in reducing the R_K uncertainty to $\mathcal{O}(1\%)$ as there are no enhanced $\mathcal{O}(\alpha)\ln\frac{m_\ell}{m_B}$ logarithms (logs) beyond scalar QED [3] and charmonium resonances are under control for $q^2 < 6\,\mathrm{GeV}^2$ [4].

process dependent Wilson lines [19, 20]. In lattice Monte Carlo simulations, hadrons are described by either gauge variant or gauge invariant interpolating operators (on which we comment at the end of section 4.1.1). No method exists for perturbative approaches with interpolating operators for charged mesons.[2] It is the aim of this paper to fill this gap.

This work is organised as follows. In section 2, some preliminary materials such as the problem of gauge variance and the universal infrared (IR) logs are discussed. In section 3, we introduce the idea of the long distance B-meson as part of the modified gauge invariant interpolating operator. In section 3.2, it is shown and argued that its LSZ-factor is IR-finite. In section 4, we establish the connection with the Dirac dressing at $\mathcal{O}(\alpha)$, and a generalisation using iterated integrals establishes the connection to all orders. The paper ends with conclusions and discussions in section 5. In appendix A, we comment on the necessity of gauge invariant interpolating operators, in connection with the hard photon approach to $B^- \to \ell^-\bar{\nu}\gamma$. In appendix B, we briefly review the QCD sum rules approximation to the LSZ approach.

2 Preliminaries

2.1 Gauge variance of the QCD interpolating operator

Let us first discuss the problem in a pedestrian way through the example of a leptonic decay of the type $B^- \to \ell^-\bar{\nu}$. In QCD, mesons such as the B^- are interpolated by[3]

$$J_B = \bar{b}i\gamma_5 u \;, \quad Z_B = \langle B^-|J_B(0)|0\rangle = \frac{m_B^2 f_B}{(m_b+m_u)} \;, \tag{2.1}$$

where Z_B plays the rôle of the LSZ-factor, This means that the matrix element

$$\langle 0|O(x)|B^-\rangle = \frac{1}{Z_B}\lim_{p^2\to m_B^2}(m_B^2-p^2)\Pi_{OB}(p^2) \;, \tag{2.2}$$

can be extracted from the correlation function

$$\Pi_{OB}(p^2) = i\int_x e^{ixp}\langle 0|TO(x)J_B(0)|0\rangle = \int_0^\infty \frac{ds}{2\pi i}\frac{\mathrm{disc}_s\Pi_{OB}(s)}{s-p^2-i0} = \frac{\langle 0|O(x)|B^-\rangle Z_B}{m_B^2-p^2} + \dots \;, \tag{2.3}$$

since the latter satisfies a dispersion relation as indicated. In (2.3), $\mathrm{disc}_s\Pi(s) = \Pi(s+i0) - \Pi(s-i0)$ is the discontinuity across the real line, the dots stand for higher states in the spectrum and $Z_B^* = Z_B$ has been assumed. The shorthands $\int_x = \int d^4x$ and $xp = x\cdot p$, used above, are occasionally assumed hereafter.

When one considers QED, the picture is fundamentally disturbed in perturbation theory since the operator J_B (or Z_B) ceases to be gauge invariant[4]

$$J_B \to e^{-i\lambda Q_B} J_B \;, \tag{2.4}$$

[2]The approach we have in mind is QCD sum rules (cf. appendix B) where the Lehmann Symanzik Zimmerman (LSZ) approach (e.g. [21]) is implemented via semi-global quark-hadron duality [22, 23].

[3]In QCD, it is advantageous to include (m_b+m_u) as a prefactor in J_B as it becomes a renormalisation group invariant quantity then. However, in QED, this will be of no use since this property is spoiled by the fact that the m_q renormalises as $e^2Q_q^2$ and thus we omit the masses in J_B.

[4]Cf. appendix A.2 for comments on the non-perturbative case.

under

$$A \to A - \partial\lambda\,, \quad q \to q e^{iQ_q\lambda}\,. \tag{2.5}$$

Hence, if there is charge ($Q_B \equiv Q_{B^-} = Q_b - Q_u = -1$ here and below), as is well-known, f_B ceases to be an observable once QED corrections are considered (e.g. [24] for a discussion for f_π). Note that (2.5) implies the $D = \partial + iA$ convention with the electric charge absorbed into the photon field A such that n photon fields correspond to $\mathcal{O}(e^n)$.

2.2 Universal infrared sensitive logs in QED

One of the main features of QED is the appearance of IR sensitive logs which can overcome the small coupling constant $\alpha = e^2/4\pi \approx 1/137$ and a fair amount is known about them. In particular, their physics is dictated and controlled by gauge invariance and thus complications are to be expected when gauge invariance is not manifest. One may distinguish two classes of logs: first, the so-called (hard) collinear logs, which arise from (charged) particles ℓ^- with small mass, allowing for collinearity with the photon up to $\mathcal{O}(\hat{m}_\ell^2)$ and resulting in sizeable $\mathcal{O}(\alpha)\ln\hat{m}_\ell$-terms (hatted quantities are divided by m_B hereafter). Second, there are soft and soft-collinear logs of the form $\mathcal{O}(\alpha)\ln\hat{m}_\gamma$ and $\mathcal{O}(\alpha)\ln\hat{m}_\gamma\ln\hat{m}_\ell$ which are true IR divergences but turn into $\mathcal{O}(\alpha)\ln\hat{\delta}$ and $\mathcal{O}(\alpha)\ln\hat{\delta}\ln\hat{m}_\ell$ when the photon emission, of $E_\gamma < \delta$, is added. Aspects of resummation of these logs are known [25, 26] but it is rather their degree of independence of the structure (or *universality*) that is of interest to us. Soft and soft-collinear logs are universal since the soft photons cannot resolve the structure of the mesons. For hard-collinear logs, the situation is not as transparent as photon energies can be as large as the kinematics allow for. It turns out that gauge invariance and the KLN-theorem (cancellation of all real and virtual IR-logs in the $m_\ell \to 0$ limit, in the photon inclusive case) are sufficient premises to show that there are no further hard-collinear logs of the form $\mathcal{O}(\alpha)\ln\hat{m}_\ell$ [3]. In other words, structure-dependent $\ln\hat{m}_\ell$ terms are subleading, either in $\mathcal{O}(\alpha)\hat{m}_\ell^2\ln\hat{m}_\ell$ or $\mathcal{O}(\alpha^2)\ln\hat{m}_\ell$, both of which are negligible.[5]

However, when the leading order (LO) process is $\mathcal{O}(m_\ell^2)$-suppressed, the theorem does not apply as then real and virtual contributions are not linked by the KLN-theorem [27]. This is precisely the case for $B^- \to \ell^-\bar{\nu}$ enabled by V-A interactions, as in the Standard Model (SM). These non-universal structure-dependent logs complicate the investigation of the validity of the approach. However, we can easily bypass this issue by resorting to an S-P interaction

$$\mathcal{L}^{(S-P)}_{B^-\to\ell^-\bar{\nu}} = g_{S-P}\,\bar{u}(1-\gamma_5)b\,\bar{\ell}(1-\gamma_5)\nu\,, \tag{2.6}$$

which is not $\mathcal{O}(m_\ell^2)$-suppressed. Hence, the hard-collinear logs are universal and, in particular, reproducible from the splitting function since the KLN-theorem applies [27]. We stress that the reasoning for choosing an S-P interaction that it allows us to test whether or not our method is capable of reproducing universal collinear logs. In summary, quoting

[5] This does not forbid other relevant and interesting structure-dependent effects such as the $m_b/\Lambda_{\mathrm{QCD}}$-enhancement found in $B_s \to \mu\mu$ [8]. In $B^- \to \ell^-\bar{\nu}$ such effects might be absent because the equation of motion of the lepton, that is the helicity suppression, work out in different ways.

JHEP11(2022)101

almost verbatim from section 3.2.1 of that reference, one has

$$\Gamma(B \to \ell\bar{\nu}(\gamma)) = \Gamma(B \to \ell\bar{\nu})^{(0)} \left(1 + \frac{\alpha}{4\pi} \left(F_{\rm soft}(\hat{m}_\ell, 2\hat{\delta}) + F_{\rm coll}(\hat{\delta}) \ln \hat{m}_\ell + \text{non-log} \right) \right) , \quad (2.7)$$

where the soft factor is

$$F_{\rm soft}(x, y) = -\left(4\frac{1+x^2}{1-x^2} \ln x^2 + 8 \right) \ln y \, , \quad (2.8)$$

and the (hard) collinear part, reproducible from the splitting function, reads

$$F_{\rm coll}(\hat{\delta}) = -4 \left(\frac{3}{2} - 2\hat{\delta}(2 - \hat{\delta}) \right) . \quad (2.9)$$

This has been backed up by an explicit computation [28]. We note that in the photon inclusive limit, $2\hat{\delta} \to 1 - \hat{m}_\ell^2$, which implies that $F_{\rm coll}(\hat{\delta}) \to \mathcal{O}(m_\ell^2)$ as required by the KLN-theorem since these logs are not suppressed by a factor of m_ℓ^2 in the rate (2.7).

The essential starting point of this paper is the observation that for the gauge variant interpolating current J_B (2.1), these universal logs are not reproduced in a perturbative computation. We shall see how to remedy it and how to interpret it in due course.

3 The long distance B-meson as a scalar field Φ_B

It is well-known that off-shell correlation functions are not gauge invariant, be it in QED or QCD, and this is at the heart of the issue raised in the introduction; namely, that the universal IR-logs are not reproduced when computing with the interpolating operator J_B (2.1). On the other hand, in scalar QED (point-like approximation), no such problems occur since the external particles can all be put on-shell. It is thus tempting to cure both, gauge invariance and the universality problem, by introducing a long distance (on-shell) B-meson in terms of a scalar field Φ_B of mass m_B as follows

$$\mathcal{J}_B^{(0)} \equiv J_B \Phi_B \, , \quad \mathcal{Z}_B^{(0)} \equiv \langle B^- | \mathcal{J}_B^{(0)} | \Phi_{B^-} \rangle \, . \quad (3.1)$$

The matrix element $\mathcal{Z}_B^{(0)}$ takes on the rôle of the LSZ-factor and its IR-finiteness is discussed in section 3.2. The explicit gauge invariance of $\mathcal{J}_B^{(0)}$ (or $\mathcal{Z}_B^{(0)}$), as opposed to J_B (2.4), is guaranteed

$$\mathcal{J}_B^{(0)} \to e^{i\lambda(Q_{\Phi_B} - Q_B)} \mathcal{J}_B^{(0)} |_{Q_B = Q_{\Phi_B}} = \mathcal{J}_B^{(0)} \, , \quad (3.2)$$

by choosing $|\Phi_{B^-}\rangle$ to have the same charge as $|B^-\rangle$; rendering $\mathcal{J}_B^{(0)}$ charge neutral. Our master formula for computing the decay rate is then

$$\Gamma_\delta(B^- \to \ell^-\bar{\nu}(\gamma)) = \frac{1}{|\mathcal{Z}_B^{(0)}|^2} \times \int_\delta d\Phi_\gamma |\mathcal{Z}_B^{(0)} \mathcal{A}(B^- \to \ell^-\bar{\nu}(\gamma))|^2 \, , \quad (3.3)$$

where both terms, the LSZ-factor $|\mathcal{Z}_B^{(0)}|^2$ and the integrand, are computed separately, and $\int_\delta d\Phi_\gamma$ is the integral over the photon phase space with $E_\gamma < \delta$ (cf. [3] for more detail). The amplitude squared is given by

$$|\mathcal{A}(B^- \to \ell^-\bar{\nu}(\gamma))|^2 = |\mathcal{A}(B^- \to \ell^-\bar{\nu})|^2 \delta(\Phi_\gamma) + |\mathcal{A}(B^- \to \ell^-\bar{\nu}\gamma)|^2 \, , \quad (3.4)$$

JHEP11(2022)101

where $\delta(\Phi_\gamma)$ is a delta function in the photon variables as appropriate for the virtual contribution. This is the famous Bloch-Nordsieck mechanism at work which bypasses the QED IR-problem of charged particles. As previously mentioned, the Φ_{B^-}-particle can be considered as the long distance version of the B-meson which splits into its partons at the $\mathcal{J}_B^{(0)}$-vertex. While being appealing, this idea should be met with scepticism at first. Its validation proceeds in several steps. The reproduction of the IR-sensitive logs from the diagrams in section 3.1 (numerator in (3.3)), the IR-finiteness of the LSZ-factor $\mathcal{Z}_B^{(0)}$ in section 3.2 (denominator in (3.3)) and the reinterpretation in terms non-local operators in section 4.

3.1 The main process

In this section, we describe how the main process, by which we mean everything in (3.3) but the LSZ-factor, is computed. We depart from the following correlation function (with $\mathcal{L}_W$, a shorthand for the weak Lagrangian, see (2.6))[6]

$$\begin{aligned}\Pi^{(\gamma)}(p_B^2, p_{\Phi_B}^2) &= i\int_x e^{ixr}\langle \ell\bar{\nu}(\gamma)|T\mathcal{J}_B^{(0)}(x)(-\mathcal{L}_W(0))|\Phi_B(p_{\Phi_B})\rangle \\ &= \int \frac{ds}{2\pi i}\frac{\mathrm{disc}_s[\Pi^{(\gamma)}(s,p_{\Phi_B}^2)]}{s-p_B^2-i0} = \frac{\mathcal{Z}_B^{(0)}\,\mathcal{A}(B^-\to\ell^-\bar{\nu}(\gamma))}{m_B^2-p_B^2} + \dots\,, \end{aligned} \tag{3.5}$$

where $r \equiv p_{\Phi_B} - p_B$ is introduced in order to distinguish the p_{Φ_B}- and the p_B-momenta, even though both are to be set on-shell (to m_B^2) in the end.[7] For p_{Φ_B}, this is straightforward

$$\Pi^{(\gamma)}(p_B^2, m_B^2) = \lim_{p_{\Phi_B}^2\to m_B^2}(m_B^2 - p_{\Phi_B}^2)\, i^2\int_{x,z} e^{i(xr-zp_{\Phi_B})}\langle \ell\bar{\nu}(\gamma)|T\Phi_B^\dagger(z)\mathcal{J}_B^{(0)}(x)\mathcal{L}_{\mathrm{W}}(0)|0\rangle\,, \tag{3.6}$$

since it plays the rôle of an elementary particle. The formal definition of the matrix element (times the LSZ-factor) is then obtained from (3.5) as

$$\mathcal{Z}_B^{(0)}\,\mathcal{A}(B^-\to\ell^-\bar{\nu}(\gamma)) = \lim_{p_B^2\to m_B^2}(m_B^2-p_B^2)\Pi^{(\gamma)}(p_B^2,m_B^2)\,. \tag{3.7}$$

We stress that (3.7) serves only as a formal definition of the matrix element since in practice, as is well-known, it is impossible to extract a bound state pole with perturbative methods, since bound states are non-perturbative.

The real emission diagrams are depicted in figure 1 and the computation of their discontinuities is straightforward. In practice, the main challenge is to compute the discontinuity of the virtual diagrams of the type shown in figure 2. We have performed this task by using Cutkosky rules as the virtual diagrams involve two loops and have a considerable number of scales. The results, with more details to be reported in [28], are the following:

1. All universal collinear logs (2.7) are reproduced *separately* for the virtual and the real rates. They originate from the sum of all $b\bar{u}$-cuts as the sum of all $b\bar{u}\gamma$-cuts is free from collinear logs (in the S-P case).

[6] Since we invoke the Bloch-Nordsieck mechanism, we may ignore that the virtual and the real emission part of the B-meson is not a well-isolated state.

[7] The r-momentum is auxiliary and momenta are to be chosen such that its effect disappears from the final result. This is rather straightforward to implement [28].

JHEP11(2022)101

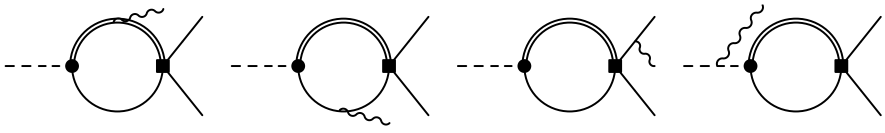

Figure 1. Diagrams contributing to $\Pi^{(\gamma)}(p_B^2, p_{\Phi_B}^2)$ in (3.5) (i.e. the radiative or real emission part). The last diagram is specific to the Φ_B-particle.

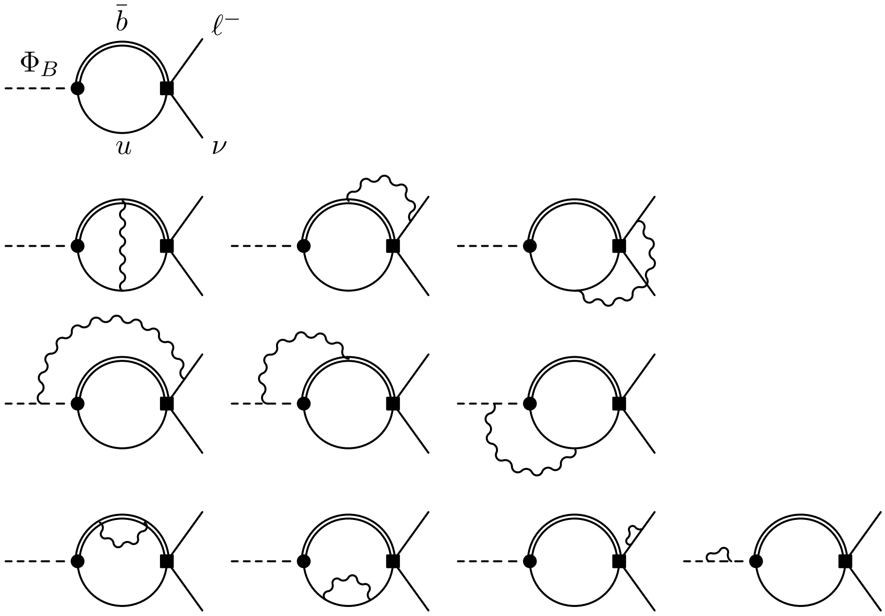

Figure 2. Diagrams contributing to $\Pi(p_B^2, p_{\Phi_B}^2)$ in (3.5) (ie. the non-radiative part, hence no (γ) superscript). Top line is the LO diagram and the third line and the last diagram are specific to the Φ_B-particle.

2. The universal soft (and soft-collinear) logs, given in (2.8), are equally reproduced and emerge as $\ln \hat{\delta}$ and $\ln \hat{\delta} \ln \hat{m}_\ell$ terms respectively.[8] In order to reproduce the soft logs the auxiliary Φ_B is crucial. Its on-shellness gives rise to the correct soft-structure in the integrand.

3. Unphysical IR divergences in $\ln m_u$ and $\ln m_\gamma$, of the collinear and soft type, cancel for the sum of all cuts. We note that this must be the case since the corresponding momentum p_B is off-shell and IR-finiteness follows from the Kinoshita-Poggio-Quinn theorem [29].

Let us remark to this end that taking all the cuts is what is usually done in the case of virtual QCD computations. However, in the case of hard photon emission, $B^- \to \ell^- \bar{\nu}\gamma$, where the photon is energetic (or non-soft), the procedure has been a different one in the literature for many decades. Why this is a valid procedure is explained in appendix A.1.

[8]Of course, the real and virtual rates contain soft-divergences, which have to be regularised (e.g. dimensional or photon mass regularisation). The split of real and virtual soft divergences is equally universal in the sense that $\ln \delta \to \ln m_\gamma|_{\text{virtual}} - \ln m_\gamma|_{\text{real}}$ restores $\ln m_\gamma$-terms.

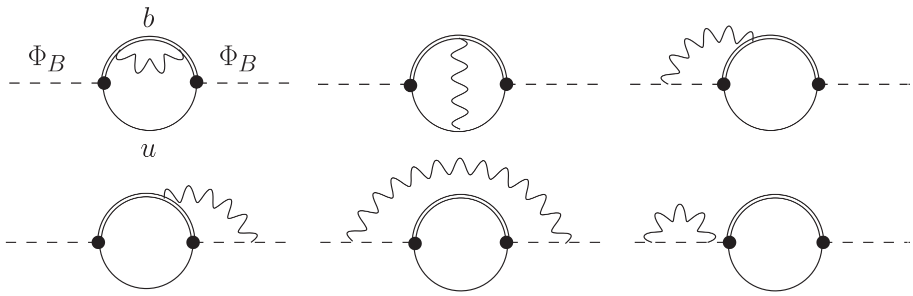

Figure 3. Diagrams contributing to $C(p_B^2, p_{\Phi_B}^2)$ (3.8), that is $|\mathcal{Z}_B^{(0)}|^2$ (3.9), where three diagrams with the photon coupling to the u-quarks are omitted as they are completely analogous to the b-quark ones.

3.2 The LSZ-factor is infrared finite

The LSZ-factor (3.1) can be extracted from the following diagonal correlation function

$$\begin{aligned} C(p_B^2, p_{\Phi_B}^2) &= i \int_x e^{ixr} \langle \Phi_B(p_{\Phi_B}) | T \mathcal{J}_B^{(0)}(x) \mathcal{J}_B^{(0)\,\dagger}(0) | \Phi_B(p_{\Phi_B}) \rangle \\ &= \int \frac{ds}{2\pi i} \frac{\mathrm{disc}_s C(s, m_{\Phi_B}^2)}{s - p_B^2 - i0} = \frac{|\mathcal{Z}_B^{(0)}|^2}{m_B^2 - p_B^2} + \dots , \end{aligned} \tag{3.8}$$

where, as before, the dots stand for higher states and this time we do not show the LSZ procedure for the Φ_B-particle explicitly, as it is straightforward. The quantity of interest is then determined from (3.8)

$$|\mathcal{Z}_B^{(0)}|^2 = \lim_{p_B^2 \to m_B^2} (m_B^2 - p_B^2) C(p_B^2, m_B^2) \,. \tag{3.9}$$

The computation proceeds in the same way as for the main process and the diagrams are shown in figure 3. One may be concerned as to whether the correlation function (or its discontinuity) are IR-finite as the Φ_B-particle is on-shell. Fortunately, $|\mathcal{Z}_B^{(0)}|^2$ turns out to be IR-finite and this follows from a physical argument. We may interpret $|\mathcal{Z}_B^{(0)}|^2$, via the optical theorem, as an inclusive decay rate of $\Phi_B(p_B) \to \bar{b} q X_0(r)$ induced by the hypothetical effective Lagrangian "$\mathcal{L}_{\text{eff}} = \mathcal{J}_B^{(0)} X_0$" where X_0 is a neutral particle (of momenta r, which decouples when $r \to 0$). Hence, by virtue of the KLN-theorem, which is based on unitarity, we know that its discontinuity must be IR-finite (also in the $m_u \to 0$ limit). We have checked that this is true by an explicit computation. Once more, it is important that one takes the sum of all cuts as individual cuts are IR divergent.

3.3 Summary of the basic interpolating operator approach

In summary, since the numerator reproduces all universal IR-sensitive logs and the denominator is IR-finite, this strongly suggests that the proposed procedure is correct. In particular, the IR-finiteness of $\mathcal{Z}_B^{(0)}$ means that the expression (3.3) has "forgotten" about its interpolating operator, as required, since it is an auxiliary in the LSZ formalism. The incorporation for several particles is straightforward from the viewpoint of the interpolating operators; one can add as many as one desires to. The same applies to non-scalar

JHEP11(2022)101

particles; for a proton one adds a scalar Φ_P and not a spin $\frac{1}{2}$-particle. The $\mathcal{O}(E_\gamma^0)$ term in Low's theorem (A.1), related to spin, is reproduced from the spinor in the form factor decomposition and is entirely kinematical.

4 Relation to non-local operators

There are gauge invariant formulations of QED, which are functionals of the photon field. These date back to the work of Dirac in 1955 [30][9] and Mandelstam in 1962 [32] where the photon field is integrated over spacetime and a spacelike path respectively. We first review the Dirac dressing in section 4.1, including the concept of dual gauges in section 4.1.1. In section 4.1.2 we show how to embed our approach at $\mathcal{O}(\alpha)$ into it. In section 4.2, the all order equivalence is established, going beyond the Dirac dressing, using iterated integrals.

4.1 Dirac dressing

One may introduce a gauge (compensating) factor $U_{\mathcal{I}}^{(P)}(x)$

$$U_{\mathcal{I}}^{(P)}(x) \equiv e^{iQ_P \int d^4y A_\mu(y) \mathcal{I}^\mu(x-y)} , \quad \partial \cdot \mathcal{I} = \delta^{(4)}(x) , \tag{4.1}$$

which is a functional of the photon field A and a current $\mathcal{I}$. The latter has no direct relation to the electromagnetic current but it is required to satisfy the differential equation above and vanishing boundary condition at infinity. There are many solutions to this equation and that will be the point of discussion soon. First, let us observe that

$$\psi_{\mathcal{I}}(x) \equiv U_{\mathcal{I}}^{(\psi)}(x)\psi(x) , \tag{4.2}$$

is gauge invariant since the gauge transformation (2.5)

$$U_{\mathcal{I}}^{(\psi)}(x) \to e^{-iQ_\psi \lambda(x)} U_{\mathcal{I}}(x) , \quad \psi(x) \to e^{iQ_\psi \lambda(x)} \psi(x) , \tag{4.3}$$

of the gauge factor and the fermion (or any other field) act to compensate each other. In effect, the gauge flux is transported by $U_{\mathcal{I}}^{(\psi)}$ to infinity where it is assumed not to matter (implicit by the imposed boundary condition).

4.1.1 Dual gauges

It is now immediate to define a gauge invariant version of J_B (2.1)

$$\mathcal{J}_B^{(D)}(\mathcal{I}, x) \equiv \bar{u}_{\mathcal{I}} i\gamma_5 b_{\mathcal{I}}(x) = J_B(x) U_{\mathcal{I}}^{(B)} , \tag{4.4}$$

by replacing the gauge variant quarks by gauge invariant ones. (Note that $U_{\mathcal{I}}^{(B)} \to e^{i\lambda Q_B} U_{\mathcal{I}}^{(B)}$). Hereafter, we suppress the subscript (B) on the gauge factor for brevity. The operator $\mathcal{J}_B^{(D)}(\mathcal{I}, x)$ is now a functional of $\mathcal{I}$. This raises the question of whether specific choices are more convenient than others and or even more legitimate. Let us first

[9]This formulation has been taken up by lattice groups [12] with C^*-boundary conditions, originally introduced for studying monopole condensation [31], since the usual periodic boundary conditions are not compatible with it.

JHEP11(2022)101

set aside the latter point. It turns out that for a given $\mathcal{I}$, one can often choose a gauge for which the gauge factor becomes trivial i.e. $U_{\mathcal{I}} = 1$. We may think of this in terms of the following equivalence or duality

$$\mathcal{J}_B^{(D)}(\mathcal{I}_{\text{gauge}}) \to J_B|_{\text{gauge}} \,, \tag{4.5}$$

where "gauge" is now an index for a specific current $\mathcal{I}$ and the subscript after the vertical bar on the right hand side indicates that the computation is to be performed in the specific gauge. This calls for examples, for which we will choose the Coulomb and Lorenz gauges (for the further example of the axial gauge, we refer the reader to [12] where these aspects are nicely discussed).

- *The Coulomb gauge:* here, the current $\mathcal{I}$, satisfying the differential equation (4.1), is

$$\mathcal{I}^0_{\text{Coulomb}}(x) = 0 \,, \quad \mathcal{I}^k_{\text{Coulomb}}(x) = -\delta(x_0)\partial^k\varphi(\vec{x}) \,, \quad \vec{\partial}^2\varphi(\vec{x}) = \delta^{(3)}(x) \,, \tag{4.6}$$

  ($k = 1, 2, 3$) where $\varphi(x)$ is the solution of the differential equation compatible with the boundary condition for $\mathcal{I}$. Indices are interpreted as Minkowski ones and $\vec{x} \cdot \vec{y} = \sum_{i=1}^3 x^i y^i$. The gauge factor may be integrated by parts to

$$U_{\mathcal{I}_{\text{Coulomb}}}(x) = e^{iQ_B \int d^3y\, \vec{\partial}\cdot\vec{A}(y)\varphi(\vec{x}-\vec{y})}|_{\vec{\partial}\cdot\vec{A}=0} \to 1 \,, \tag{4.7}$$

  and trivialises in the Coulomb gauge $\vec{\partial} \cdot \vec{A} = 0$.

- *The Lorenz gauge:* in this case, the current $\mathcal{I}$, satisfying the differential equation, is

$$\mathcal{I}^\mu_{\text{Lorenz}}(x) = \partial^\mu\varphi(x) \,, \quad \partial^2\varphi(x) = \delta^{(4)}(x) \,. \tag{4.8}$$

  Integrating by parts, the gauge factor reads

$$U_{\mathcal{I}_{\text{Lorenz}}}(x) = e^{iQ_B \int d^4y\, \partial\cdot A(y)\varphi(x-y)}|_{\partial\cdot A=0} \to 1 \,, \tag{4.9}$$

  and trivialises in the Lorenz/Landau gauge, $\partial \cdot A = 0$.[10]

We wish to stress that the choice of gauge here is nothing but a computational trick or a matter of convenience. The element of complexity in the gauge factor $U_{\mathcal{I}_{\text{gauge}}}$ is moved into computing with the gauge variant operator J_B in a specific gauge. These two effects of gauge dependence act to compensate each other.

Let us now return to the question, alluded to before, of whether all choices of $\mathcal{I}$ are equally valid. We would think that the answer to this question ought to be yes in approaches with an exact LSZ formula. However, if the LSZ formula is approached in the sense of duality as in QCD sum rules (cf. appendix B), this is not the case as it turns out that neither the Coulomb nor the Lorenz gauge current reproduce the universal IR-logs in (2.7). This was explicitly verified using the gauge factor $U_{\mathcal{I}}$.

[10]Since the gauge fixing term reads $\mathcal{L}_{\text{gauge}} = \frac{1}{2\xi}(\partial \cdot A)^2$, the Landau gauge $\xi = 0$ and the Lorenz gauge condition are equivalent (at least in perturbation theory).

JHEP11(2022)101

4.1.2 The Φ_B-particle in Dirac dressing

Hence, the natural question is whether our approach which is gauge invariant can be captured in this formalism with a specific current $\mathcal{I}$. The following expression achieves this task

$$\mathcal{I}^{\mu}_{\Phi_B}(x) = (\partial - 2ip)^{\mu} e^{ixp}\varphi(x) \ , \quad (\partial^2 + m_B^2)\varphi(x) = \delta^{(4)}(x) \ , \tag{4.10}$$

where $p \equiv p_{\Phi_B}$ for brevity and on-shell momentum ($p^2 = m_B^2$). As a solution to the differential equation (4.1) with the appropriate boundary condition, the Feynman propagator $\varphi(x) = i\Delta_F(x, m_B^2)$ is chosen. The gauge factor integrates by part to

$$U_{\mathcal{I}_{\Phi_B}}(x,p) = e^{iQ_B \int d^4y\, e^{i(x-y)p}\Delta_F(x-y, m_B^2)(i\partial + 2p)\cdot A(y)} \ , \tag{4.11}$$

a most familiar form. Namely, the exponent becomes the Feynman rule for scalar QED with the scalar being our Φ_B-particle! In fact, a hint of this possibility was given by the Lorenz gauge case (4.8) which, however, corresponds to the massless propagator with zero momentum insertion ($p_\mu = 0$). Here, we have in effect extended this mechanism to the massive propagator with a non-zero momentum. For clarity, let us quote the corresponding interpolating operator

$$\mathcal{J}_B^{(D)}(x,p) \equiv J_B(x) U_{\mathcal{I}_{\Phi_B}}(x,p) \ , \tag{4.12}$$

where the superscript (D) stands for Dirac. A natural question, in view the discussion in section 4.1.1, is whether there exists a dual gauge (that trivialises the gauge factor (4.11))? The answer is yes,

$$U_{\mathcal{I}_{\Phi_B}}(x,p)\big|_{(i\partial+2p)\cdot A=0} \to 1 \ , \tag{4.13}$$

which is a peculiar axial gauge for which the photon propagator in momentum space assumes the form

$$\Delta_{\mu\nu}(k)\Big|_{\Phi_B-\text{gauge}} = \frac{1}{k^2}\left(-g_{\mu\nu} - n^2\frac{k_\mu k_\nu}{(n\cdot k)^2} + \frac{k_{\{\mu}n_{\nu\}}}{n\cdot k}\right) \ , \quad n = k + 2p \ , \tag{4.14}$$

with $k_{\{\mu}n_{\nu\}} = k_\mu n_\nu + k_\nu n_\mu$, and $n^\mu \Delta_{\mu\nu} = 0$ as required.

4.2 Iterated integral approach

It is clear that the form in (4.11) is not suitable for higher order computations, or already the Φ_B self-energy correction. Matters can be improved by writing an expression with *iterated* integrals. For that purpose, let us define the following kernel

$$K(z,y) \equiv iQ_B\, e^{izp}\Delta_F(z, m_B^2)(i\partial + 2p)\cdot A(y) \ , \tag{4.15}$$

suppressing the p and A dependence in K. Then, the improved and final version reads

$$\mathcal{J}_B(x,p) \equiv J_B(x) V_{\mathcal{I}_{\Phi_B}}(x,p) \ , \tag{4.16}$$

where

$$V_{\mathcal{I}_{\Phi_B}}(x,p) = 1 + \sum_{n\geq 1}\int d^4y_1 \ldots d^4y_n K(x-y_1, y_1)\ldots K(y_{n-1}-y_n, y_n) \ , \tag{4.17}$$

JHEP11(2022)101

consists of the iterated kernels K. In essence, this formula is the Dyson series for the Φ_B-particle where the propagators have been contracted already and this is the reason why the $1/n!$-factor from the exponential has disappeared! To establish the gauge transformation, $V_{\mathcal{I}_{\Phi_B}}(x) \to e^{iQ_B\lambda(x)} V_{\mathcal{I}_{\Phi_B}}(x)$, by direct computation is not a simple matter. However, it is clear that it must hold since the Φ_B-formalism is gauge invariant. In addition, we have verified the transformation law explicitly up to fourth order, witnessing intricate cancellations.

The $\mathcal{J}_B$ interpolating operator is the most transparent and most generally valid version obtained in this paper as it clarifies a number of questions. For example, does the Φ_B-particle need to be included into the running of the fine structure constant α? The answer is negative since it just "lives" inside the factor $V_{\mathcal{I}}$ and does not figure in the Lagrangian of the theory. This means that there is no coupling to charged fermions other than through the interpolating operator itself. As such it serves as a justification for the rules applied previously. In summary we thus have the following relation

$$\mathcal{Z}_B = \mathcal{Z}_B^{(0)} = \mathcal{Z}_B^{(D)} + \mathcal{O}(\alpha^2) \,, \tag{4.18}$$

formulated in terms of the respective LSZ-factors.[11]

5 Conclusions and discussions

In this work, a method was proposed for incorporating charged hadrons via gauge invariant interpolating operators for perturbative methods such as QCD sum rules. Technically, this consists of adding the long distance field Φ_B to the gauge variant operator J_B (2.1), that is $\mathcal{J}_B^{(0)} \equiv J_B \Phi_B$ (3.1). Intuitively, Φ_B takes on the rôle of the long distance B-meson splitting into its two valence partons $\bar{u}$ and b, thereby resolving the dilemma that bound states (e.g. hadrons) are beyond perturbation theory, but essential for infrared-sensitive physics. Formally, Φ_B solves two linked problems at once: $J_B \to \mathcal{J}_B^{(0)}$ becomes gauge invariant since it is charge neutral, and the universal logs (cf. (2.7) and the end of section 3.1) are reproduced. The main formula for computing processes is given in eq. (3.3), where both parts, the numerator and denominator, are computed separately. The modified LSZ-factor $\mathcal{Z}_B^{(0)}$ is gauge invariant and IR-finite which can be argued to hold on grounds of the KLN-theorem. Together with the reproduction of the universal IR-logs, this consists of the cornerstone in validating the approach.

In section 4, we established the link of the method to the Dirac dressing of charged fields to $\mathcal{O}(e^2)$, $\mathcal{J}_B^{(D)}$, which can be found in eqs. (4.12) and (4.11). An improved version $\mathcal{J}_B$, valid to all orders, generalising the Dirac dressing by using iterated integrals has been given in eqs. (4.16) and (4.17). Reassuringly, this generalisation makes it clear that the Φ_B-particle does not contribute to the running of the fine structure constant α since it

[11]The $\mathcal{J}_B$-formulation is related to the coherent state framework in the sense that the soft logs (not the hard-collinear log) are reproduced. This is achieved by taking the coherent state function to be the eikonal factor $\omega_\mu \propto p_\mu/(p \cdot k)$ which defines the coherent state $|\omega\rangle \propto \exp(\int d\Phi_\gamma \omega^\mu a_\mu^\dagger)|0\rangle$ with $a_\mu^\dagger$ being the photon creation operator [33] (and [27] for a more complete set of references). Again, this has to be the case since soft resummation is equivalent to the coherent state approach at the leading log level.

JHEP11(2022)101

does not appear in the Lagrangian of the theory. The dual gauge, trivialising the gauge factor, has been identified as a peculiar axial gauge, cf. eqs. (4.13) and (4.14).

Note that the method generalises to any number of particles and any types of spins with remarks at the end of section 3.3. One can add for each charged particle an operator of the form (4.16). However, one can use the trick of the trivialising gauge only once. Explicit results of the computation for leptonic decays, which necessitate one interpolating operator only, including numerics, are to follow in a forthcoming publication [28].

Acknowledgments

We would to thank Martin Beneke, Luigi Del Debbio, Matteo Di Carlo, Giulio Falcioni, Einan Gardi, Max Hansen, Anton Ilderton Agostino Patella, Antonin Portelli and further participants of the "QED in Weak Decays" workshop in Edinburgh for useful discussions and feedback. In particular, we acknowledge the input of Matt Rowe to this work in terms of proofreading, discussions and computations RZ is supported by an STFC Consolidated Grant, ST/P0000630/1. SN is supported by the GLUODYNAMICS project funded by the "P2IO LabEx (ANR-10-LABX-0038)" in the framework "Investissements d'Avenir" (ANR-11-IDEX-0003-01) managed by the Agence Nationale de la Recherche (ANR), France.

A On the necessity of gauge invariant interpolating operators

In this appendix, we comment under which circumstances interpolating operators for charged mesons are necessary or not. This seems mandatory since processes with charged hadrons have been considered in the literature using gauge variant interpolating operators. This includes i) $B^- \to \ell^- \bar{\nu}\gamma$ where γ is a hard photon, to be discussed in appendix A.1, and ii) leptonic decays in lattice Monte Carlo simulations, to be discussed in appendix A.2.

A.1 Relation to computations of $B^- \to \ell^- \bar{\nu}\gamma$ with a hard photon

There is some good tradition in using QED gauge dependent interpolating operators J_B (2.1) for $B^- \to \ell^- \bar{\nu}\gamma$ in QCD sum rule approaches; e.g at $\mathcal{O}(\alpha_s^0)$ [34, 35] and $\mathcal{O}(\alpha_s)$ [36] or for the $g_{B^- B^{*-}\gamma}$ coupling at $\mathcal{O}(\alpha_s^0)$ [35] and $\mathcal{O}(\alpha_s)$ [37]. This raises the obvious question of how the issues raised, at the beginning of the paper, were avoided.

First and foremost, at $\mathcal{O}(e)$, that is, for a single photon emission, these observables are formally analogous to $B^- \to \ell^- \bar{\nu}\rho^0(k)$ and $g_{B^- B^{*-}\rho^0}$ respectively. The main point is that the ρ^0 or the hard photon (say $E_\gamma \geq \Lambda_{\mathrm{QCD}}$) are considered as separate particles and formally, this implies that $\{q^2, p_B^2, k^2\}$ are the independent kinematic variables, referred to as the hard photon approach.[12] The situation is illustrated in figure 4 with further comments in the caption.

Computing $\mathcal{O}(\alpha_s)$ corrections to $B^- \to \ell^- \bar{\nu}\gamma$ and $g_{B^- B^{*-}\gamma}$ is demanding, but straightforward, because J_B is QCD gauge invariant. However, complications arise if we were to

[12] In the soft photon approach, pursued in this work, $\{p_B \cdot k, p_B^2, k^2\}$ are the independent variables. More comments are to follow further below.

JHEP11(2022)101

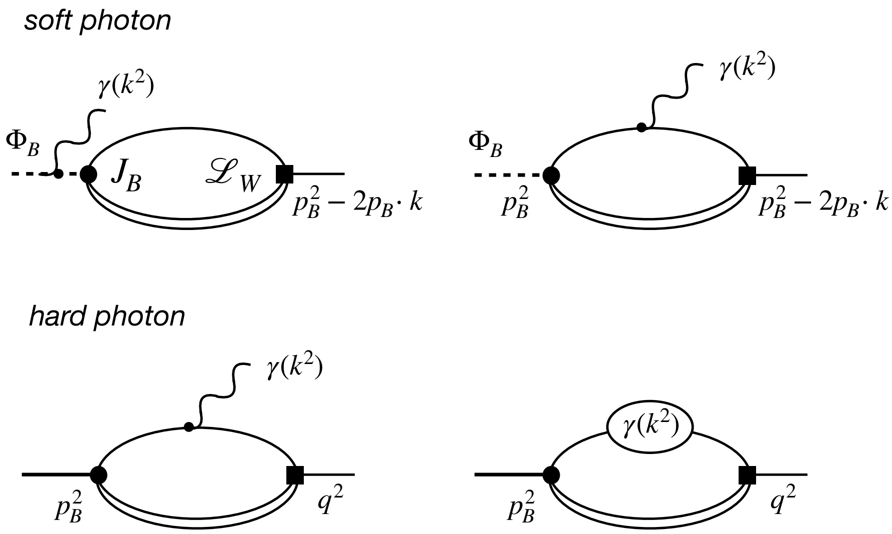

Figure 4. Comparison of soft and hard photon approaches. In the soft photon approach (top diagrams), $q^2 \to p_B^2 - 2p_B \cdot k$ (since $k^2 = 0$) and $p_B \cdot k$ becomes an independent variable. Top left (right) diagram correspond to the Φ_B (quarks)-term in (A.5). Note that the top left diagram reproduces the Low term and the top right diagram is finite as $p_B \cdot k \to 0$. In the hard photon approach (bottom diagrams), q^2 is an independent variable. The Low term is produced by the bottom left diagram (cutting in p_B^2), while the bottom right diagram probes the structure. In particular, the blob is the photon distribution amplitude (DA) and is generated by a sum over intermediate mesons ρ^0, ω, ϕ with quantum numbers of the photon $J^{PC} = 1^{--}$. For an elaborate discussion of this viewpoint, see appendix A of [38]. The mappings of the diagrams between the two approaches are as follows: top left $\subset$ bottom left, bottom right $\subset$ top right. The first relation follows from the fact that the point-like interaction on the top-left does not "know" anything about the non-perturbative $\rho - \gamma$ conversion that the photon DA represents and this also implies the second relation.

compute $\mathcal{O}(\alpha)$ radiative corrections as J_B is QED gauge variant. In that case, the introduction of the gauge invariant interpolating operator becomes, in our opinion, a necessity in perturbation theory. One should regard $B^- \to \ell^- \bar{\nu}\gamma$ with the hard photon as a LO process, and it is only its radiative corrections that necessitate the introduction of the soft photon (to complement the virtual corrections). This is in line with the picture of coherent states (e.g. [27] and relevant references therein).

It is still an interesting question as to how $B^- \to \ell^- \bar{\nu}\gamma$ at $\mathcal{O}(e)$ with gauge invariant interpolating operator $\mathcal{J}_B$ reduces to the case of the gauge variant operator J_B; in particular, of how the Low terms emerge, giving rise to the universal IR-logs for which we had to introduce the Φ_B-particle. *Low's theorem* [39], quoted with the same convention as in [27], states that adding a real photon to a transition $\alpha \to \beta$

$$\langle \beta\gamma(k,\lambda)|S|\alpha\rangle = \frac{c_{-1}}{E_\gamma} + c_0 + c_1 E_\gamma + \mathcal{O}(E_\gamma^2) \; , \tag{A.1}$$

JHEP11(2022)101

the two first terms in an E_γ-expansion are universal and given by

$$\frac{c_{-1}}{E_\gamma} = \sum_j \hat{Q}_j \frac{\epsilon^*(k,\lambda)\cdot\hat{p}_j}{k\cdot\hat{p}_j - i0}\langle\beta|S|\alpha\rangle\ , \quad c_0 = -i\sum_j \hat{Q}_j \frac{\epsilon^*_\mu(k,\lambda)k_\nu J_j^{\mu\nu}}{k\cdot\hat{p}_j - i0}\langle\beta|S|\alpha\rangle\ . \tag{A.2}$$

Above, $J_j^{\mu\nu} = i\hat{p}_j^{[\mu}\partial^{\nu]}_{\hat{p}_j}$ is the orbital angular momentum operator (and square brackets denote anti-symmetrisation). Hatted quantities are plus(minus) its value for outgoing(incoming) particles.

To further simplify matters, we consider the S-P interaction (2.6), in which case there are no $B\to\gamma$ form factors by helicity conservation and it all reduces to the Low-term corresponding to the emission from the B-meson (and the charged lepton of course). More concretely, at LO, the amplitude factorises

$$\begin{aligned}\mathcal{A}^{S-P}_{B^-\to\ell^-\bar{\nu}\gamma} &= \langle\gamma\ell^-\bar{\nu}| - \mathcal{L}^{(S-P)}_{B^-\to\ell^-\bar{\nu}}|B^-\rangle \\ &= -g_{S-P}\langle\gamma|\bar{u}(1-\gamma_5)b|B^-\rangle\langle\ell^-\bar{\nu}|\ell(1-\gamma_5)\nu|0\rangle + \dots\ ,\end{aligned} \tag{A.3}$$

where g_{S-P} is an irrelevant constant for our purposes and the dots stand for photon emission from the lepton. We focus on the first term which, by Low's theorem, gives

$$\mathcal{A}^{S-P}_{B\to\gamma} \equiv -im_b\langle\gamma|\bar{u}(1-\gamma_5)b|B^-(p_B)\rangle = -eQ_B\frac{p_B\cdot\epsilon^*}{p_B\cdot k}\mathcal{A}_{LO} = -\frac{2eQ_Bm_B^2f_B}{m_B^2-q^2}(p_B\cdot\epsilon^*)\ , \tag{A.4}$$

where $\mathcal{A}_{LO} = m_B^2 f_B$ (having set $m_u=0$), $p_B\cdot k = \frac{1}{2}(m_B^2-q^2)$, ϵ is the photon's polarisation vector, and by parity, only the γ_5-part contributes. Two remarks are in order: i) as this is an on-shell matrix element, hence $p_B^2 = m_B^2$ ii) the expression (A.4) is exact, as stated before.

Now, we would like to see how this works out in our approach (with gauge invariant interpolating operator). The correlation function (3.5) evaluates to

$$\Pi^{(\gamma)}(p_B^2, p_{\Phi_B}^2, q^2) \propto eQ_B\left(\left[\frac{\Pi_P(q^2)}{m_B^2-q^2}\right]_{\Phi_B} + \left[\frac{\Pi_P(p_B^2)-\Pi_P(q^2)}{p_B^2-q^2}\right]_{\text{quarks}}\right)(p_B\cdot\epsilon^*) + \dots\ , \tag{A.5}$$

where the dots once more stand for the photon emission from the lepton (and $(p_B - p_{\Phi_B})\cdot\epsilon^*$-terms which have to be dropped as they are unphysical). The first term in the $p_B\cdot\epsilon^*$-structure corresponds to emission from the Φ_B-particle, the second term to emission from the quarks and $\Pi_P(s)$ is the following 2-point function

$$\Pi_P(p^2) = i\,m_b^2\int_x e^{ipx}\langle 0|TJ_B(x)J_B^\dagger(0)|0\rangle\ . \tag{A.6}$$

which is further scrutinised in section B. Note that the extra factor of J_B arises from the quark part of the weak Lagrangian. The quark emission term in (A.5) can be established without computation as being the unique solution to the QED Ward identity. This goes hand in hand with the statement that (A.4) is exact. Now, we have all the information in order to investigate the differences between the two approaches.

JHEP11(2022)101

- *Hard photon approach* $\{q^2, p_B^2, k^2\}$: in this case q^2 is considered an independent variable and the discontinuity in p_B^2 is given by

$$\mathrm{disc}_{p_B^2}\Pi^{(\gamma)}(p_B^2, p_{\Phi_B}^2, q^2) \propto \frac{\mathrm{disc}_{p_B^2}\Pi_P(p_B^2)}{p_B^2 - q^2} \;, \tag{A.7}$$

which reproduces the Low-term (A.4) to the extent that $p_B^2 \to m_B^2$, which holds in QCD and approximately for QCD sum rules at the level of quark hadron duality as noticed in [36] (and cf. appendix B). The latter is a sufficiently good approximation as long as q^2 is not too close to m_B^2 which is the premise of the hard photon QCD sum rule approach.

- *Soft photon approach* $\{p_B{\cdot}k, p_B^2, k^2\}$: it is characterised by $E_\gamma \ll \Lambda_{\rm QCD}$ and it makes more sense to expand around E_γ (or better its covariant form $p_B \cdot k$). Eq. (A.5), omitting its arguments, then becomes

$$\Pi^{(\gamma)} \propto eQ_B \left(\left[\frac{\Pi_P(q^2)}{2p_{\Phi_B}{\cdot}k} \right] + \left[\frac{\Pi_P(p_B^2) - \Pi_P(q^2)}{2p_B \cdot k} \right] \right) \Bigg|_{q^2 \to p_B^2 - 2p_B\cdot k} (p_B \cdot \epsilon^*) + \dots \;, \tag{A.8}$$

and formally we traded q^2 for $p_B \cdot k$. Note that, at the end, $p_B \cdot k$ is set equal to $p_{\Phi_B} \cdot k = E_\gamma m_B$ The first thing to notice is that in the $k \to 0$ limit, the second term becomes $\Pi'_P(p_B^2)$, the derivative of the 2-point function, and contributes to c_0, but does not reproduce the c_{-1}-term in (A.1).[13] This rôle is reserved the Φ_B-term! This highlights the necessity of introducing the Φ_B-particle in this approach. Most importantly, the two terms in $\Pi_P(q^2)$ exactly cancel each other

$$\mathrm{disc}_{p_B^2}\Pi^{(\gamma)}|_{q^2 \to p_B^2 - 2p_B\cdot k} \propto \frac{\mathrm{disc}_{p_B^2}\Pi_P(p_B^2)}{2p_B{\cdot}k} \;, \tag{A.9}$$

and the Low term appears in its exact form (A.4) (after the LSZ formula in p_B^2 is applied).

The example of the S-P interaction almost appears a bit too simple to illustrate the point but in fact it is not. In the V-A case, there would simply be many other terms contributing to the structures in (A.1) other than the Low-term (e.g. [36]).

An interesting question that one could raise is the following: how can taking cuts in p_B^2 in the hard photon approach be equivalent to taking cuts in p_B^2 itself and an extra cut in $q^2 = p_B^2 - 2p_B \cdot k$ in the soft photon approach? The answer is that for $s_0 - m_b^2 < m_B^2 - q^2$, where s_0 is the (effective) continuum threshold, this extra cut does not actually contribute to the sum rule (cf. (B.6)). This translates to $q^2 < 14\,\mathrm{GeV}^2$ for typical values of $s_0 = 35\,\mathrm{GeV}^2$ and $m_b = 4.6\,\mathrm{GeV}$ (pole or kinetic scheme m_b-mass). This is what is usually assumed in the light-cone expansion indeed (e.g. [36]). Hence for $q^2 > 14\,\mathrm{GeV}^2$, or well-above, the hard photon approach gradually breaks down and the soft photon variables become appropriate.

[13]This is in accordance with the Kinoshita-Poggio-Quinn-theorem (cf. [27] for references) which states that in renormalisable theories, off-shell correlation functions are free from IR singularities for non-exceptional momenta.

JHEP11(2022)101

A.2 Exact LSZ formula and gauge variant interpolating operators

Let us comment on the necessity of gauge invariant interpolating operators. If one aims only at $\mathcal{O}(\alpha)$ in a decay process and one has an exact LSZ formula, then it would seem possible to work with gauge variant interpolating operators for hadrons. This is because the hadrons are the QCD hadrons (not corrected by QED) and those states are well-isolated in the spectrum. The Euclidean correlation function then assumes the form

$$Z_B(\text{gauge}) \times \text{amplitude} \times e^{-E_B t_E} + \dots \,, \tag{A.10}$$

where the dots stand for exponentially suppressed terms (cf. (B.9)) and Z_B corresponds to the gauge variant LSZ-factor of the B-interpolating operator in use. The exact LSZ formula emerges in the limit of infinite Euclidean time separation of the meson source. In this case, the exponentially suppressed terms disappear as $t_E \to \infty$ and the sole gauge dependence is in Z_B and can be cancelled by computing it from an appropriate correlation function. This is the idea underlying the QED$_L$ [10] and the QED$_{m_\gamma}$ [11] lattice approaches.

When aiming for corrections beyond $\mathcal{O}(\alpha)$, matters are more delicate since charged states are not isolated anymore (QED IR-problem, see [27] for references) and an explicit gauge invariant formulation seems more appropriate. This is the idea behind the C^*-boundary method [12]. So far, this method has only been applied to hadronic masses and the specifics for (leptonic) decay rates have not been proposed to date.

B Brief review of the LSZ formalism and QCD sum rule approach

In this appendix, we briefly review the LSZ formalism (e.g. [21]) itself and how it is handled in QCD sum rules [22]. We do so by considering the 2-point function in eq. (A.6) relevant to $B^- \to \ell^-\bar{\nu}\gamma$ for S-P interactions. In QCD and perturbative QCD (pQCD), the most important terms for our considerations are

$$\Pi_P(s)\Big|_{\text{QCD}} = \frac{m_B^4 f_B^2}{s - m_B^2} + \dots \,, \tag{B.1}$$

$$\Pi_P(s)\Big|_{\text{pQCD}} = \frac{N_c}{8\pi^2} m_b^2 \left(1 - \frac{m_b^2}{s}\right)^2 s \, \ln(m_b^2 - s) + \dots \,, \tag{B.2}$$

where N_c are the number of colours. The dots stand for higher states in the spectrum in (B.1) and non-logarithmic terms, condensate terms and $\mathcal{O}(\alpha_s)$-contributions in (B.2) (for pQCD, cf. [37] for explicit results). In the LSZ approach, repeating the steps in (2.2), one would extract the amplitude $\mathcal{A}_{\text{LO}}$, referred to below (A.4), by

$$\mathcal{A}_{\text{LO}} = \frac{1}{Z_B'} \lim_{p_B^2 \to m_B^2} (m_B^2 - p_B^2) \Pi_P(p_B^2)\Big|_{\text{QCD}} = m_B^2 f_B \,. \tag{B.3}$$

Here, $Z_B' = m_b Z_B = m_B^2 f_B$ (cf. also (2.1)) and the dots in (B.1) vanish as they do not have a pole in $(p_B^2 - m_B^2)$. Let us consider this aspect by a dispersive representation ("s.t." stands for subtraction terms)

$$\Pi_P(p^2) = \int_0^\infty ds \frac{\rho_P(s)}{s - p^2 - i0} + \text{ s.t.} \,, \tag{B.4}$$

with $2\pi i \rho_P(s) = \mathrm{disc}_s \Pi_P(s)$. From (B.1), one gets

$$\begin{aligned}
\rho_P(s)\Big|_{\mathrm{QCD}} &= m_B^4 f_B^2 \delta(s - m_B^2) + \dots \,, \\
\rho_P(s)\Big|_{\mathrm{pQCD}} &= \frac{N_c}{8\pi^2} m_b^2 \left(1 - \frac{m_b^2}{s}\right)^2 s\, \theta(s - m_B^2) + \dots \,.
\end{aligned} \tag{B.5}$$

Subtraction terms are eliminated by a Borel transform which maps any polynomial in s to zero and $1/(s - p^2) \to \exp(-s/M^2)/M^2$ (with M^2 the Borel mass). We may then rewrite (B.3)

$$\mathcal{A}'_{\mathrm{LO}}[\rho_P] = \frac{1}{Z_B} \int_{\mathrm{cut}}^{s_0} ds\, e^{(m_B^2 - s)/M^2} \rho_P(s) \,, \tag{B.6}$$

where "cut" marks the start of the discontinuity and s_0 is just below the onset of the first excited states which are of the order of $(m_B + 2m_\pi)^2$ to $(m_B + m_\rho)^2$. The difference between QCD and QCD sum rules is now most clear

$$\begin{aligned}
\mathcal{A}'_{\mathrm{LO}}\left[\rho_P\Big|_{\mathrm{QCD}}\right] &= \mathcal{A}_{\mathrm{LO}} \,, \qquad \text{exact} \,, \\
\mathcal{A}'_{\mathrm{LO}}\left[\rho_P\Big|_{\mathrm{pQCD}}\right] &\approx \mathcal{A}_{\mathrm{LO}} \,, \qquad \text{QCD sum rule} \,,
\end{aligned} \tag{B.7}$$

as it reduces to which density is in use. The approximation made can be quantified by[14]

$$\int_{s_0}^{\infty} ds\, e^{(m_B^2 - s)/M^2} \rho_P(s)\Big|_{\mathrm{pQCD}} \approx \int_{s_0}^{\infty} ds\, e^{(m_B^2 - s)/M^2} \rho_P(s)\Big|_{\mathrm{QCD}} \,, \tag{B.8}$$

and is sometimes referred to as semi-global quark-hadron duality [23]. In practice, it may be expected to hold to within 30% and if the pole term dominates by 60%, this leads to an uncertainty of roughly 10% [22]. In practice, most sum rules are ratios of sum rules in fact, such as (3.3), and this effect cancels to a considerable extent. Eq. (B.8) can be expected to work well when the higher spectrum is broad, that is, if there are no further narrow resonances, which is most often the case.

At last, it is worthwhile to sketch the analogue of the LSZ formula in Euclidean field theory in which the positive frequency correlation function in the time-momentum representation is considered

$$\Pi_P^+(t_E, \vec{p}^{\,2}) = m_b^2 \int d^3x\, e^{i\vec{x}\cdot\vec{p}} \langle 0|J_B(x) J_B^\dagger(0)|0\rangle \propto (Z'_B)^2\, e^{-E_B t_E} + \dots \,. \tag{B.9}$$

Above the dots stand for exponentially suppressed terms and Z'_B has been defined below (B.3). The physical matrix element emerges in the $t_E \to \infty$ such that the suppressed terms disappear.

[14] It is tempting to take the limit $M^2 \to 0$ as then the higher states would decouple. However, the problem with this is that then the operator products expansion does not converge in that case. $M^2 \to 0$ is in some sense the analogue of infinite Euclidean time separation in lattice QCD.

References

[1] S. Bifani, S. Descotes-Genon, A. Romero Vidal and M.-H. Schune, *Review of Lepton Universality tests in B decays*, *J. Phys. G* **46** (2019) 023001 [arXiv:1809.06229] [INSPIRE].

[2] LHCb collaboration, *Tests of lepton universality using $B^0 \to K^0_S \ell^+\ell^-$ and $B^+ \to K^{*+}\ell^+\ell^-$ decays*, *Phys. Rev. Lett.* **128** (2022) 191802 [arXiv:2110.09501] [INSPIRE].

[3] G. Isidori, S. Nabeebaccus and R. Zwicky, *QED corrections in $\overline{B} \to \overline{K}\ell^+\ell^-$ at the double-differential level*, *JHEP* **12** (2020) 104 [arXiv:2009.00929] [INSPIRE].

[4] G. Isidori, D. Lancierini, S. Nabeebaccus and R. Zwicky, *QED in $\bar{B} \to \bar{K}\ell^+\ell^-$ LFU ratios: theory versus experiment, a Monte Carlo study*, *JHEP* **10** (2022) 146 [arXiv:2205.08635] [INSPIRE].

[5] V. Cirigliano, M. Knecht, H. Neufeld, H. Rupertsberger and P. Talavera, *Radiative corrections to K(l3) decays*, *Eur. Phys. J. C* **23** (2002) 121 [hep-ph/0110153] [INSPIRE].

[6] V. Cirigliano, M. Giannotti and H. Neufeld, *Electromagnetic effects in K(l3) decays*, *JHEP* **11** (2008) 006 [arXiv:0807.4507] [INSPIRE].

[7] S. Descotes-Genon and B. Moussallam, *Radiative corrections in weak semi-leptonic processes at low energy: A Two-step matching determination*, *Eur. Phys. J. C* **42** (2005) 403 [hep-ph/0505077] [INSPIRE].

[8] M. Beneke, C. Bobeth and R. Szafron, *Enhanced electromagnetic correction to the rare B-meson decay $B_{s,d} \to \mu^+\mu^-$*, *Phys. Rev. Lett.* **120** (2018) 011801 [arXiv:1708.09152] [INSPIRE].

[9] M. Beneke, C. Bobeth and R. Szafron, *Power-enhanced leading-logarithmic QED corrections to $B_q \to \mu^+\mu^-$*, *JHEP* **10** (2019) 232 [arXiv:1908.07011] [INSPIRE].

[10] N. Carrasco et al., *QED Corrections to Hadronic Processes in Lattice QCD*, *Phys. Rev. D* **91** (2015) 074506 [arXiv:1502.00257] [INSPIRE].

[11] M.G. Endres, A. Shindler, B.C. Tiburzi and A. Walker-Loud, *Massive photons: an infrared regularization scheme for lattice QCD+QED*, *Phys. Rev. Lett.* **117** (2016) 072002 [arXiv:1507.08916] [INSPIRE].

[12] B. Lucini, A. Patella, A. Ramos and N. Tantalo, *Charged hadrons in local finite-volume QED+QCD with C^* boundary conditions*, *JHEP* **02** (2016) 076 [arXiv:1509.01636] [INSPIRE].

[13] X. Feng and L. Jin, *QED self energies from lattice QCD without power-law finite-volume errors*, *Phys. Rev. D* **100** (2019) 094509 [arXiv:1812.09817] [INSPIRE].

[14] V. Lubicz, G. Martinelli, C.T. Sachrajda, F. Sanfilippo, S. Simula and N. Tantalo, *Finite-Volume QED Corrections to Decay Amplitudes in Lattice QCD*, *Phys. Rev. D* **95** (2017) 034504 [arXiv:1611.08497] [INSPIRE].

[15] D. Giusti et al., *First lattice calculation of the QED corrections to leptonic decay rates*, *Phys. Rev. Lett.* **120** (2018) 072001 [arXiv:1711.06537] [INSPIRE].

[16] M. Hansen, B. Lucini, A. Patella and N. Tantalo, *Gauge invariant determination of charged hadron masses*, *JHEP* **05** (2018) 146 [arXiv:1802.05474] [INSPIRE].

[17] M. Di Carlo et al., *Light-meson leptonic decay rates in lattice QCD+QED*, *Phys. Rev. D* **100** (2019) 034514 [arXiv:1904.08731] [INSPIRE].

[18] M.A. Clark et al., *QED with massive photons for precision physics: zero modes and first result for the hadron spectrum*, *PoS* **LATTICE2021** (2022) 281 [arXiv:2201.03251] [INSPIRE].

JHEP11(2022)101

[19] M. Beneke, P. Böer, J.-N. Toelstede and K.K. Vos, *Light-cone distribution amplitudes of light mesons with QED effects*, *JHEP* **11** (2021) 059 [arXiv:2108.05589] [INSPIRE].

[20] M. Beneke, P. Böer, J.-N. Toelstede and K.K. Vos, *Light-cone distribution amplitudes of heavy mesons with QED effects*, *JHEP* **08** (2022) 020 [arXiv:2204.09091] [INSPIRE].

[21] A. Duncan, *The Conceptual Framework of Quantum Field Theory*, Oxford University Press (2012).

[22] M.A. Shifman, A.I. Vainshtein and V.I. Zakharov, *QCD and Resonance Physics. Theoretical Foundations*, *Nucl. Phys. B* **147** (1979) 385 [INSPIRE].

[23] M.A. Shifman, *Quark hadron duality*, in *8th International Symposium on Heavy Flavor Physics*, Southampton, U.K. (1999), *Quark-hadron duality*, World Scientific (2000), pg. 1447 [hep-ph/0009131] [INSPIRE].

[24] J. Gasser and G.R.S. Zarnauskas, *On the pion decay constant*, *Phys. Lett. B* **693** (2010) 122 [arXiv:1008.3479] [INSPIRE].

[25] D.R. Yennie, S.C. Frautschi and H. Suura, *The infrared divergence phenomena and high-energy processes*, *Annals Phys.* **13** (1961) 379 [INSPIRE].

[26] E.A. Kuraev and V.S. Fadin, *On Radiative Corrections to e^+e^- Single Photon Annihilation at High-Energy*, *Sov. J. Nucl. Phys.* **41** (1985) 466 [INSPIRE].

[27] R. Zwicky, *Notes on QED Corrections in Weak Decays*, *Symmetry* **13** (2021) 2036 [arXiv:2205.06194] [INSPIRE].

[28] S. Nabeebaccus, M. Rowe and R. Zwicky, *Leptonic decays and structure-dependent QED*, in preparation.

[29] T. Muta, *Foundations of quantum chromodynamics*, second edition, *World Scientific Lecture Notes in Physics. Vol. 57*, World Scientific (1998).

[30] P.A.M. Dirac, *Gauge invariant formulation of quantum electrodynamics*, *Can. J. Phys.* **33** (1955) 650

[31] L. Polley and U.J. Wiese, *Monopole condensate and monopole mass in* U(1) *lattice gauge theory*, *Nucl. Phys. B* **356** (1991) 629 [INSPIRE].

[32] S. Mandelstam, *Quantum electrodynamics without potentials*, *Annals Phys.* **19** (1962) 1 [INSPIRE].

[33] P.P. Kulish and L.D. Faddeev, *Asymptotic conditions and infrared divergences in quantum electrodynamics*, *Theor. Math. Phys.* **4** (1970) 745 [INSPIRE].

[34] A. Ali and V.M. Braun, *Estimates of the weak annihilation contributions to the decays $B \to \rho\gamma$ and $B \to \omega\gamma$*, *Phys. Lett. B* **359** (1995) 223 [hep-ph/9506248] [INSPIRE].

[35] A. Khodjamirian, G. Stoll and D. Wyler, *Calculation of long distance effects in exclusive weak radiative decays of B meson*, *Phys. Lett. B* **358** (1995) 129 [hep-ph/9506242] [INSPIRE].

[36] T. Janowski, B. Pullin and R. Zwicky, *Charged and neutral $\overline{B}_{u,d,s} \to \gamma$ form factors from light cone sum rules at NLO*, *JHEP* **12** (2021) 008 [arXiv:2106.13616] [INSPIRE].

[37] B. Pullin and R. Zwicky, *Radiative decays of heavy-light mesons and the $f^{(T)}_{H,H^*,H_1}$ decay constants*, *JHEP* **09** (2021) 023 [arXiv:2106.13617] [INSPIRE].

[38] J. Albrecht, E. Stamou, R. Ziegler and R. Zwicky, *Flavoured axions in the tail of $B_q \to \mu^+\mu^-$ and $B \to \gamma^*$ form factors*, *JHEP* **09** (2021) 139 [arXiv:1911.05018] [INSPIRE].

[39] F.E. Low, *Scattering of light of very low frequency by systems of spin* 1/2, *Phys. Rev.* **96** (1954) 1428 [INSPIRE].