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Isospin mass differences of the B, D and K

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Abstract: We compute the electromagnetic mass difference for the B-, D- and K-mesons using QCD sum rules with double dispersion relations. For the B- and D-mesons we also compute the linear quark mass correction, whereas for the K the standard soft theorems prove more powerful. The mass differences, which have not previously been computed via a double dispersion, are fully consistent with experiment, albeit with large uncertainties.

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Contents

1 Introduction **1**

2 Electromagnetic mass difference $\Delta m_H|_{\mathrm{QED}}$ from QCD sum rules **3**
2.1 B- and D-meson with pseudoscalar operators 4
2.1.1 Numerics 6
2.2 K-meson with axial operators 7

3 Linear quark mass correction $\Delta m_H|_{m_q}$ **9**
3.1 QCD sum rule computation of $\langle \bar{H}|\bar{q}q|\bar{H}\rangle$ for $H = B, D$ 9
3.1.1 Numerics 10
3.2 $\mathrm{SU}(3)_F$ estimates of $\langle \bar{H}|\bar{q}q|\bar{H}\rangle$ for $H = B, D$ 11
3.3 Soft Goldstone estimate of $\langle L|\bar{q}q|L\rangle$ for $L = \pi, K$ 12

4 Final overview and conclusions **12**

A Variants of quark-hadron duality **13**
A.1 Weight function $\omega(s) = s$ 14
A.2 Weight function $\omega(s) = \frac{1}{s-\eta}$ 15

B Numerical input **15**
B.1 Decay constants f_B, f_D and f_K 15

C Double cuts, self energies and condensates for $\Delta m_H|_{\mathrm{QED}}$ **16**
C.1 Perturbation theory: $b - q$ diagram 16
C.2 Perturbation theory: self energies 17
C.3 Condensates 17

D Some classic results **18**
D.1 Linear quark mass dependence from Feynman-Hellman theorem 18
D.2 $\Delta m_\pi|_{\mathrm{QED}}$ from soft theorem and Weinberg sum rules 18

1 Introduction

The mass difference of charged and neutral hadrons,

$$\Delta m_H = m_{H^+} - m_{H^0}\,, \qquad H = B, D, K, \pi, p\,, \tag{1.1}$$

is an isospin breaking effect and has intrigued particle physicists from the very beginning. In particular the proton-neutron [1] and the π^+-π^0 [2] mass difference have been discussed extensively. At the microscopic level Δm_H is driven by differences in the electric charge and the mass m_q of the hadron's light valence quark $q = u, d$

$$\Delta m_B = \Delta m_B|_{\text{QED}} + \Delta m_B|_{m_q} \,. \tag{1.2}$$

The sign and the size depends on the hadron in question and QED stands for quantum electrodynamics.[1],[2] Recent lattice Monte Carlo simulations [3, 4] have verified this to a high accuracy, for light and charm mesons, by computing both the charged and the neutral mass and effectively using (1.1). Light meson splittings were also analysed in [7] using coupled Dyson-Schwinger and Bethe-Salpeter equations.

One may take a different approach and compute the two differences in (1.2) separately by using the second order perturbation theory formula (with $H = B$ for definiteness)[3]

$$\delta m_B|_{\text{QED}} = \frac{-i\alpha}{2m_B(2\pi)^3} \int d^4q \, T^{(B)}_{\mu\nu}(q)\Delta^{\mu\nu}(q) + \mathcal{O}(\alpha^2) \,, \tag{1.3}$$

with

$$\Delta m_B|_{\text{QED}} \equiv \delta m_{B^+}|_{\text{QED}} - \delta m_{B^0}|_{\text{QED}} \,, \tag{1.4}$$

known in the current algebra era [8, 9]. Above $\Delta_{\mu\nu}(q) = \frac{1}{q^2}(-g_{\mu\nu} + (1-\xi)\frac{q_\mu q_\nu}{q^2})$ is the photon propagator, $\alpha = e^2/(4\pi)$ the fine structure constant and $T^{(B)}_{\mu\nu}(q)$ is the (uncontracted) forward Compton scattering tensor,

$$T^{(B)}_{\mu\nu}(q) = i \int d^4x e^{-iq\cdot x} \langle B|Tj_\mu(x)j_\nu(0)|B\rangle \,, \tag{1.5}$$

with $j_\alpha = \sum_q Q_q \bar{q}\gamma_\alpha q$, the electromagnetic current.

In 1963, Cottingham [10] improved this formula by parameterising it in terms of form factors and relating it to structure functions. That is, by deforming the contour $q_0 \to iq_0$ and writing a dispersion representation, assessing the number of subtraction terms of the form factors thus allowing him to write the contribution as an integral over $Q^2 = -q^2 \geq 0$ and $\nu = p \cdot q/m_B$ in the physical region. This opened the gate for many phenomenological studies saturating the dispersion relation by a few terms beyond the elastic one and using high energy constraints. This is a formidable task as one requires the knowledge of a correlation function over the entire energy range akin to the situation of the vacuum polarisation for the anomalous magnetic moment. Some examples are for K, π [11, 12] using chiral perturbation theory (and large N_c), for B and D [13, 14] using heavy quark theory (and large N_c), for the proton-neutron [15] with updated fits to the structure functions and an approach to B, D, K and π using vector meson dominance [16]. Another interesting point, not unrelated, is that (1.3) requires renormalisation [17] and it was argued that it is

[1] Strictly speaking the separation (1.2) is not well-defined as it requires fixing a (quark mass) renormalisation scheme e.g. [3]. In turn this is a reason for being interested in the problem as, especially light, quark masses cannot be determined to high precision without folding in QED. This shows for example in the D-meson results in comparison between [3] and [4]. For our purposes $\Delta m_B|_{m_q}$ is as defined from (1.7).

[2] Effects due to the weak force are of $\mathcal{O}(\Lambda^2_{\text{QCD}}/m_W^2)$ with respect to QED and are thus negligible. Similar effects are relevant in the context of neutral meson mixing e.g [5, 6].

[3] Note that in the literature the notation $\Delta m_B^2 \equiv 2m_B\Delta m_B$ is also frequently used.

justified to cut-off the Q^2-integral. The divergences associated with the quark and the gluon condensate in the OPE are related to the mass and the coupling constant renormalisation at $\mathcal{O}(\alpha)$ (e.g. [18] where this spelled out). Debates about subtraction terms in dispersion representation of (1.5) are ongoing cf. [15] and the response [19].

Here we do *not* follow this phenomenological approach but evaluate (1.5) directly in Minkowski space using double dispersion relation sum rules and thus determine the mass differences from a unified framework (i.e. same hadronic input).[4] Note that the double dispersion is necessity since each B-meson requires an (approximate dispersive) LSZ procedure. To the best of our knowledge this has not been done previously with sum rules, presumably due to the subtleties of non gauge-invariant interpolating currents [23, 24]. For example, in leptonic decays this requires the introduction of a non-local interpolating operator (or an auxiliary scalar field carrying the charge to infinity) for gauge invariance and reproduction of all infrared sensitive logs [24]. However, in the case at hand this is not necessary, as verified by explicit computation, since Δm_B is an infrared safe quantity.

An efficient and transparent way to implement the first order quark mass corrections is to make use of the Feynman-Helmann theorem which gives

$$m_B^2|_{m_q} = \sum_q m_q \langle B|\bar{q}q|B\rangle + \mathcal{O}(m_q^2, m_q^2 \ln mq)\,, \tag{1.6}$$

as rederived in appendix D.1. For the difference (1.1) this gives

$$\Delta m_B\,|_{m_q} = \frac{(m_u - m_d)}{2m_B}\langle B|\bar{q}q|B\rangle + \mathcal{O}((m_u - m_d)^2)\,. \tag{1.7}$$

The matrix element $\langle B|\bar{q}q|B\rangle$ can be evaluated in the isospin degenerate limit $q = u = d$ since we work to leading order (LO). For the B- and the D-meson we compute this matrix element whereas for the Kaon and the pion a soft theorem (e.g. [25]) $\langle \pi|\bar{q}q|\pi\rangle = -\frac{2}{f_\pi^2}\langle 0|\bar{q}q|0\rangle + \mathcal{O}(m_\pi^2/m_\rho^2)$, with $f_\pi \approx 131\,\text{MeV}$, due to their pseudo-Goldstone nature, proves more effective.

In principle one could compute all the $\Delta m_B|_{m_q}$-effects with the QCD analogue of (1.3) but this would be rather inefficient and we further comment in the relevant section. Another noteworthy aspect is that we were not able to obtain stable sum rules for the pion (cf. section 2.2).

The paper is organised as follows. In section 2 the electromagnetic computation is presented, followed by the quark mass correction in section 3. We give an overview of the results and the conclusions in section 4. Comments on quark hadron duality, the numerical input. some (extra) computation and useful classic results are collected in Appendices A, C, B and D respectively.

2 Electromagnetic mass difference $\Delta m_H|_{\text{QED}}$ from QCD sum rules

The electromagnetic mass difference follows from the formula quoted in (1.3) and it is our task to evaluate this. The main theoretical challenge is to incorporate the two hadrons for

[4] This function has been evaluated for the pion on the lattice with good agreement with experiment in [20] (method in [21]) and [4, 22] (method in [18]).

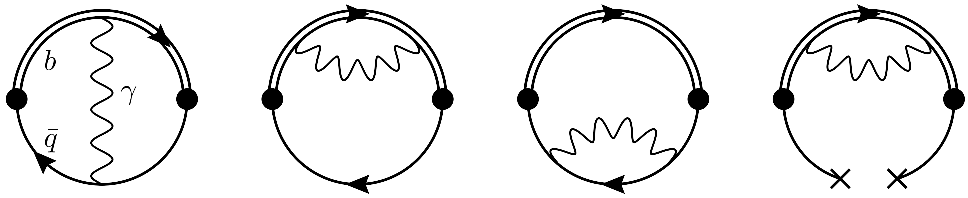

Figure 1. Diagrams contributing to the correlation function in (2.3) with the double line representing the b-quark. (left) main diagram of the Q_bQ_q mixed type. (middle) b- and q-quark self energies. (right) $\langle\bar{q}q\rangle$-condensate part to b-quark self energy. There is no corresponding part for the q-quark self energy since $\langle\bar{b}b\rangle$ is negligibly small. For the mass difference only the first one is relevant while the others are useful to obtain stable sum rules as described in the text.

which a non-perturbative method is needed. We use QCD sum rules [26] with a double dispersion relation. The first step involves the adaption of an interpolating operator. For the heavy mesons a pseudoscalar current is suitable and has proven to give good results in many other contexts. For particles of light quark masses, and Goldstone particles in particular [27], pseudoscalar interpolating operators are unsuitable as they are infested by so-called direct instantons [28].[5] We therefore discuss the heavy mesons and the K-meson separately in sections 2.1 and 2.2 respectively.

An important criteria in assessing the validity of our sum rules is the so-called daughter sum rule which we consider worthwhile to present now. In the simple single dispersion relation case this criteria reads

$$m_B^2(s_0, M^2) = \int_{\text{cut}}^{s_0} e^{-s/M^2} \rho(s) s ds / (\int_{\text{cut}}^{s_0} e^{-s/M^2} \rho(s) ds) \,, \tag{2.1}$$

where M^2 is the Borel parameter, the "cut" marks the onset of physical states, $\rho(s) = r_B \delta(s - m_B^2) + \ldots$ is the spectral density and the dots stand for states above the continuum threshold s_0. Formally, the residue r_B drops out in the ratio. In practice $\rho(s)$ is a continuous function in partonic computations and eq. (2.1) should be seen as a self-consistency criteria for an s_0 in the range of $(m_B + 2m_\pi)^2$ of $(m_B + 4m_\pi)^2$. If that is the case then eq. (2.1) can be used to fix the central value of s_0.

2.1 *B*- and *D*-meson with pseudoscalar operators

As motivated at the beginning of the section, the default choice for heavy-light 0^- meson interpolating operators are

$$J_B = m_+ \bar{b} i \gamma_5 q \,, \quad Z_B \equiv \langle \bar{B} | J_B | 0 \rangle = m_B^2 f_B \,, \quad m_+ \equiv (m_b + m_q) \,. \tag{2.2}$$

In determining (1.3), one of the main challenges, is that the momenta for the two B-meson is degenerate. We bypass this problem by introducing an auxiliary momentum r into one of

[5]For the heavy mesons axial interpolating operators are unsuitable because the 1^+ states are relatively low, e.g. for the $J^P = 0^-$ B-meson with $m_B \approx 5.28\,\text{GeV}$ there is a 1^+ $B_1(5721)$ with $m_{B_1} \approx 5.72\,\text{GeV}$. This is too close to the two pion threshold and even below the typical continuum threshold $s_0 \approx (6\,\text{GeV})^2$ assumed for the pseudoscalar operators.

JHEP06(2023)089

the currents and let it flow out at one of the two interpolating operators. Concretely we start from

$$\Gamma_{qq'}(p^2, \tilde{p}^2) = c\, i^3 \int_{x,y,z,q} e^{i(\tilde{p}z - ipy - (q+r)x)} \langle 0|T J_B^\dagger(z) j_\mu(x) j_\nu(0) J_B(y)|0\rangle \Delta^{\mu\nu}(q)|_{Q_q Q_{q'}}$$
$$= \int_0^\infty ds \int_0^\infty d\tilde{s} \frac{\rho_{\Gamma_{qq'}}(s,\tilde{s})}{(s-p^2)(\tilde{s}-\tilde{p}^2)} = \frac{Z_B^2 \delta_{qq'} m_B}{(m_B^2 - p^2)(m_B^2 - \tilde{p}^2)} + \dots , \tag{2.3}$$

with $c \equiv \frac{-i\alpha}{2m_B(2\pi)^3}$, $\tilde{p} = p + r$, shorthands $xp = x \cdot p$, $\int_{q,x} = \int d^4q d^4x$ and the density is given by

$$(2\pi i)^2 \rho_{\Gamma_{qq'}}(s,\tilde{s}) = \mathrm{disc}_{s,\tilde{s}}[\Gamma_{qq'}(s,\tilde{s})] , \tag{2.4}$$

the double discontinuity with further relevant explanations at the end of the section. The quantity $\Delta_{qq'} m_B$ denotes the part proportional to the $Q_q Q_{q'}$-charges. Of course the auxiliary momentum r has to disappear from the final result. This is achieved by the on-shell condition "$\tilde{p}^2 = p^2$" and is implemented in practice by treating them equally (p-$\tilde{p}$ symmetry) and requiring the daughter sum rule to be satisfied reasonably well. The QCD sum rule is then given by

$$\delta_{qq'} m_B = \frac{1}{Z_B^2} \int_{m_+^2}^{\bar{\delta}^{(a)}(m_+^2)} ds\, e^{\frac{(m_B^2 - s)}{M^2}} \int_{m_+^2}^{\bar{\delta}^{(a)}(s)} d\tilde{s}\, e^{\frac{(m_B^2 - \tilde{s})}{M^2}} \rho_{\Gamma_{qq'}}(s,\tilde{s}) , \tag{2.5}$$

where M^2 is the Borel parameter from the Borel transformation and the $\bar{\delta}^{(a)}$ is the continuum threshold

$$\bar{\delta}^{(a)}(s) = 2^{1/a}\sigma_0 \left(1 - \left(\frac{s}{2^{1/a}\sigma_0}\right)^a\right)^{1/a} , \tag{2.6}$$

which is complicated for double dispersion sum rules [29]. Here it is implemented as in [30] but simplified since the two hadrons are identical implying $M^2 \to 2\hat{M}^2$ and $\tilde{s}_0 = \tilde{t}_0 = \sigma_0^{(a)} 2^{1/a}$ (allowing for elimination of those parameters). The number $\sigma_0 \approx 35\,\mathrm{GeV}^2$ takes on the rôle of s_0 in (2.1) and we shall use the notation $s_0 \equiv \sigma_0$ hereafter for reasons of familiarity. The parameter a is a model-parameter and the independence of the result is a measure of the quality of the result itself.

Let us turn to the computation of which further details are given in appendix C. In perturbation theory there is the diagram connecting the q- to the b-quark and the self energies. We focus on the former, as it is numerically dominant, and present the self energies and the condensate contribution in appendix C. The computation can be done analytically and we obtain the following compact result for the density

$$\rho_{\Gamma_{bq}} = \frac{N_c \alpha Q_q Q_b m_+^2}{32\pi^3 m_B} \cdot \frac{\sqrt{\lambda\tilde{\lambda}}}{s\tilde{s}} \left(A + \frac{B}{\mathsf{b}} \ln\left(\frac{\mathsf{a}+\mathsf{b}}{\mathsf{a}-\mathsf{b}}\right)\right) , \tag{2.7}$$

where

$$\mathsf{a} = m_q^2 - \frac{1}{4\sqrt{s\tilde{s}}}(s\tilde{s} + (m_+ m_-)^2) + \left\{q \leftrightarrow b\right\} , \qquad \mathsf{b} = \frac{1}{2}\sqrt{\frac{\lambda\tilde{\lambda}}{s\tilde{s}}} , \qquad A = m_-^2 ,$$
$$B = \left\{ Y\tilde{Y} s\tilde{s} + \frac{1}{2} m_q^2 \sqrt{s\tilde{s}}(Y + \tilde{Y}) - \frac{1}{4} m_-^2 \left(s + \tilde{s} + 4m_b m_q + 2m_q^2\right) - \frac{1}{4} m_+^2 \sqrt{s\tilde{s}} \right\} + \left\{q \leftrightarrow b\right\} ,$$

with further abbreviations

$$m_\pm = m_b \pm m_q\,, \quad \lambda = \lambda(s, m_b^2, m_q^2)\,, \quad Y = \frac{s - m_+ m_-}{2s}\,, \tag{2.8}$$

$\lambda(x,y,z) = x^2 + y^2 + z^2 - 2xy - 2xz - 2yz$ is the Källén function and in the tilde quantities $\tilde{Y}$ and $\tilde{\lambda}$ we have $s \to \tilde{s}$.

A few words about the computation. We have taken the discontinuity in (2.4) using Cutkosky rules. A crucial point is that we do not cut the photon propagator as this would be a QED correction to the B-meson state and does not contribute to (1.3). This amends the meaning of (2.4).

Let us turn to the usage of the auxiliary momentum r in the context of double dispersion sum rules. First we note that this is different to a form factor computation, e.g. $F^{\pi\to\pi}(q^2)$ [31], where the momentum transfer naturally takes on the rôle of this variable. It is closer to $\Delta F = 2$ matrix elements as there is no momentum transfer but the flavour contractions naturally lead to a symmetric configuration (e.g. [32]) which is more straightforward. In fact since our procedure (2.3) artificially breaks the bq-symmetry, $\mathtt{a}$ and B turn out to be non-symmetric whereas $\mathtt{b}$ and A remain symmetric. This has to be remedied by the following substitution

$$\mathtt{a} \to \frac{1}{2}(\mathtt{a} + \mathtt{a}|_{b\leftrightarrow q})\,, \quad B \to \frac{1}{2}(B + B|_{b\leftrightarrow q})\,, \tag{2.9}$$

which is apparent from the way the Cutkosky cuts work out. We have performed the computation in general gauge. Of course $\Gamma_{qq'}$ is gauge dependent but as stated earlier its discontinuity in the bq-quark lines are not. This is the case since the particles are put on the mass shell and it is important that the quantity is infrared safe. Otherwise, as previously stated, one needs to introduce extra machinery [24].

2.1.1 Numerics

Our numerics have three cornerstones, the hadronic input parameters in table 2, the daughter sum rule (2.1) and the choice of a mass scheme for m_b. Whereas there is nothing to say about point one, the others are in need of some explanation. We start with the B-meson case. The daughter sum rule constrains the sum rule parameters: the continuum threshold s_0 and the Borel parameter M^2. Additional constraints, defining the Borel window, are the convergence of the condensate expansion and keeping the B-pole term dominant versus the continuum contribution [26]. Let us turn to the question of the mass scheme which is not independent of the second point. We consider the pole-, the kinetic- and the $\overline{\text{MS}}$-scheme. In the pole scheme the b,c-quark self energy contributions (perturbative and condensate, diagrams 2 and 4 in figure 1) vanish and the sum rules are not stable, that is no Borel window, and we therefore discard it. For the $\overline{\text{MS}}$-scheme the b-quark self energies are dominant with the b-q contribution comparable to the condensates. Since these contributions cancel in the observable Δm, this scheme is not ideal either and we therefore drop it. Hence we are left with the kinetic scheme for the b-quark which shows good properties as for the $B \to \gamma$ form factor [33] and the $g_{BB*\gamma}$-couplings [30]. For the

c-quark the self energies are not dominant and we use the $\overline{\text{MS}}$-scheme, also because the kinetic-scheme has proven unsuitable in for $g_{DD*\gamma}$ [30].

As stated above the daughter sum rule (2.1) is used to fix s_0. For that purpose it is instructive to define the normalised ratio

$$\mathrm{U}(s_0, M^2) \equiv \frac{1}{m_B^2} \cdot m_B^2(s_0, M^2)\,, \tag{2.10}$$

of the sum rule value over the experimental one which has to be close to unity for self-consistency of the approach. This leads to[6]

$$\{s_0, \hat{M}^2\}_B = \{35.2(1.0), 2.6(0.5)\}\,\text{GeV}^2\,, \qquad \{s_0, \hat{M}^2\}_D = \{5.5(1), 1.0(0.25)\}\,\text{GeV}^2\,, \tag{2.11}$$

for which

$$\mathrm{U}(s_0 \pm 1\,\text{GeV}^2, M^2)_{\Delta m_B|_{\text{QED}}} = 1 \pm 0.01\,, \quad \mathrm{U}(s_0 \pm 0.1\,\text{GeV}^2, M^2)_{\Delta m_D|_{\text{QED}}} = 1 \pm 0.01\,.$$

Using the input parameters in table 2 (with $m_b^{\text{kin}}(1\,\text{GeV}), \bar{m}_c(\bar{m}_c)$) and the $f_{B,D}$ sum rule to LO (cf. appendix B.1) for the Z_B-factor we get

$$\Delta m_B|_{\text{QED}} = +1.58^{+0.26}_{-0.23}\,\text{MeV}\,, \qquad \Delta m_D|_{\text{QED}} = +2.25^{+0.89}_{-0.52}\,\text{MeV}\,, \tag{2.12}$$

where the error is obtained by adding the individual errors in quadrature. The dominant error is due to the heavy quark mass $m_{b(c)}$ (50-60%). The Borel mass M^2 and duality parameters a each contribute a 20-25% uncertainty. The error in a is quantified by taking the standard deviation of the results with $a \in [\frac{1}{2}, 1, 2, \infty]$. The errors for the D-meson are larger reflecting the generically inferior quality of the sum rule.

2.2 K-meson with axial operators

As explained at the beginning of this section pseudo Goldstone bosons cannot be interpolated by pseudoscalar operators and one therefore resorts to axial ones

$$A_\mu = \bar{q}\,\gamma_\mu\gamma_5\,s\,, \quad \langle 0|A_\mu|K(p)\rangle = ip_\mu f_K\,. \tag{2.13}$$

The correlation function corresponding to (2.3) assumes the form

$$\begin{aligned}\Gamma^{\alpha\beta}_{qq'}(p^2, \tilde{p}^2) &= ci^3 \int_q \int_{x,y,z} e^{i(\tilde{p}z - py - (q+r)x)} \langle 0|TA^\alpha(z) j_\mu(x) j_\nu(0) A^{\dagger\,\beta}(y)|0\rangle \Delta^{\mu\nu}(q)|_{Q_q Q'_q} \\ &= g_{\alpha\beta}\Gamma^{(0)}_{qq'} + p_\alpha p_\beta \Gamma^{(2)}_{qq'} + \mathcal{O}(r)\ldots\,,\end{aligned} \tag{2.14}$$

where the $\mathcal{O}(r)$-terms are not of interest to us. The decisive information is in the $p_\alpha p_\beta$-term which takes on the form

$$\Gamma^{(2)}_{qq'} = \frac{f_K^2 \delta_{qq'} m}{(m_K^2 - p^2)(m_K^2 - \tilde{p}^2)} + \ldots\,, \tag{2.15}$$

[6]Note that in our case the s_0 is isospin-independent since we work in the linear approximation. When estimating the QCD isospin breaking to decay constant this is a different matter cf. [34].

in a hadronic representation where the dots represent higher states in the spectrum (which includes the K^*-meson in this case).

Let us turn to the computation which involves some practical matters. Computing the double discontinuity of $\Gamma^{(2)}_{qq'}$ is laborious as there are open Lorentz indices. One may though obtain the same information from a linear combination of (2.3) and (2.14) with contracted indices. It follows from Ward identities that ($d = 4$)

$$\Gamma^{(2)}(s,s) = \frac{1}{s^2(1-d)} \left(s\Gamma^{\alpha}_{\alpha}(s,s) - d\,\Gamma(s,s) \right) , \tag{2.16}$$

where we omitted the qq'-subscript for brevity and have set $s = \tilde{s}$. The generalisation to the $s \neq \tilde{s}$ is in principle ambiguous but fortunately the differences are not that sizeable. Concretely we use

$$\Gamma^{(2)}(s,\tilde{s}) = \frac{1}{s\tilde{s}(1-d)} \left(\frac{1}{2}(s+\tilde{s})\Gamma^{\alpha}_{\alpha}(s,\tilde{s}) - d\,\Gamma(s,\tilde{s}) \right) , \tag{2.17}$$

and the analogous expression of (2.7) is lengthy for the Kaon and is given in a Mathematica ancillary notebook attached to the arXiv version.

Changing the prescription (2.17) by $\frac{1}{2}(s+\tilde{s}) \to \sqrt{s\tilde{s}}$ results in a 15%-change which is sizeable but not extremely large and well within the error. In addition we use a weight function $1/s\tilde{s}$ as described in appendix A.2 as otherwise the daughter sum rule is off by at least a factor of two which is very large in view of how well it works in all other cases.

Proceeding as before we obtain the following values

$$\{s_0, \hat{M}^2\}_K = \{0.7(1), 0.95(0.5)\}\,\mathrm{GeV}^2 , \qquad \mathrm{U}(s_0 \pm 0.1, M^2)_{\Delta m_K|_{\mathrm{QED}}} = 1.00 \pm 0.10 , \tag{2.18}$$

for the sum rule parameters and the daughter sum rule (2.10). Using the input parameters in table 2, the f_K sum rule to LO (cf. appendix B.1) and (2.18) we get[7]

$$\Delta m_K|_{\mathrm{QED}} = +1.85^{+0.42}_{-0.66}\,\mathrm{MeV} . \tag{2.19}$$

Scale dependent quantities are evaluated at $\mu = 2\,\mathrm{GeV}$. The uncertainty again comes from adding individual errors in quadrature. The dominant uncertainty (75%) comes from the m_s mass with the remaining uncertainty due to the duality parameter a in (2.6).

As stated in the introduction, the pion proved more difficult. That is we were not able to find stable sum rules satisfying the daughter sum rule for reasonable values of the continuum threshold.[8] We believe that is due to its small mass m_π which is considerably below the other hadronic masses. Conversely the Kaon mass, while being a pseudo-Goldstone, is much closer to the other hadrons (due to m_s being close to Λ_{QCD}).

[7]The error estimates presented are found by varying the input parameters to the sum rule in a procedural way. By not rounding the error digits we do not imply that the error is that precise. The uncertainties should thus be taken as only indicative of the error.

[8]The extra disconnected diagram for the π^0, e.g. [20], is small since the γ_5 generates a Levi-Civita tensor which enforces two extra loops. This is reflected in the smallness of the lattice result [20] and also by the fact that the LO chiral Lagrangian does not contribute to π^0 (cf. appendix D.2).

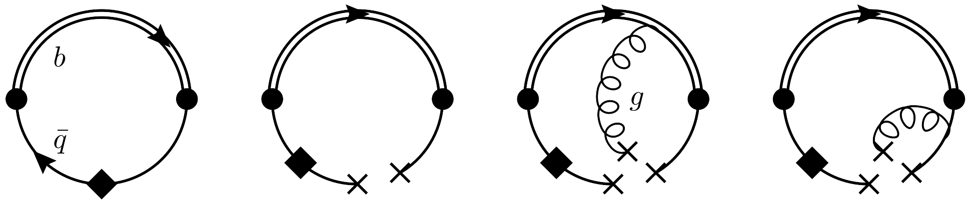

Figure 2. Diagrams contributing to the matrix element $\langle B|\bar{q}q|B\rangle$. They are analogous to the ones in figure 1 but the square blob denotes the insertion of the $\bar{q}q$-operator. Perturbation theory is minimal and the quark condensate diagram is the main contribution. The mixed condensate diagrams $\langle\bar{q}Gq\rangle$ are mainly useful to stabilise the sum rule.

3 Linear quark mass correction $\Delta m_H|_{m_q}$

As stated in the introduction (and cf. appendix D.1) the $\mathcal{O}(m_q)$-corrections are governed by $\langle H|\bar{q}q|H\rangle$ (1.7). For the B, D-meson we compute this matrix element from QCD sum rules in section 3.1, using similar techniques as for the QED correction, and for light mesons we resort to soft theorems cf. section 3.3 as the corresponding sum rules are inferior.

3.1 QCD sum rule computation of $\langle\bar{H}|\bar{q}q|\bar{H}\rangle$ for $H = B, D$

In order to anticipate the hierarchy of diagrams shown in figure 2 it is worthwhile to contemplate on the heavy quark behaviour. The matrix element scales like ($H = B$) for definiteness).

$$\langle B|\bar{q}q|B\rangle = \mathcal{O}(m_b)\,, \tag{3.1}$$

for relativistically normalised states, $\langle B(p)|B(q)\rangle = 2E_B(\vec{p})(2\pi)^3\delta^{(3)}(\vec{p}-\vec{q})$, due to the factor $E_B = \mathcal{O}(m_b)$. On the one hand, the operator $\bar{q}q$ demands a chirality flip in perturbation theory and this cannot come from the m_b-mass since the latter is entirely kinematic as we have just established. On the other hand the condensate contribution itself $\langle\bar{q}q\rangle$ does not require this flip and is therefore unsuppressed and numerically leading.

To do the computation we start from the following correlation function

$$\Pi(p^2,\tilde{p}^2,r) = i^2\int_{y,z} e^{i(\tilde{p}z-py-xr)}\langle 0|TJ_B^\dagger(z)(\bar{q}q)(x)J_B(y)|0\rangle\,, \tag{3.2}$$

where J_B has been defined in (2.2) and the auxiliary momentum r takes on the same rôle as before. The double dispersion relation of the correlation functions reads

$$\Pi(p^2,\tilde{p}^2,r) = \int\frac{ds d\tilde{s}\,\rho_\Pi(s,\tilde{s})}{(s-p^2-i0)(\tilde{s}-\tilde{p}^2-i0)} = \frac{Z_B^2\langle\bar{B}|\bar{q}q|\bar{B}\rangle}{(m_B^2-p^2)(m_B^2-\tilde{p}^2)} + \ldots\,, \tag{3.3}$$

with $(2\pi i)^2\rho_\Pi(s,\tilde{s}) = \mathrm{disc}_{s,\tilde{s}}[\Pi(s,\tilde{s})]$, and the matrix element is then given by

$$\langle\bar{B}|\bar{q}q|\bar{B}\rangle = \frac{1}{Z_B^2}\int_{m_+^2}^{\bar{\delta}^{(a)}(m_+^2)} ds\, e^{\frac{(m_B^2-s)}{M^2}}\int_{m_+^2}^{\bar{\delta}^{(a)}(s)} d\tilde{s}\, e^{\frac{(m_B^2-\tilde{s})}{M^2}}\rho_\Pi(s,\tilde{s})\,, \tag{3.4}$$

with $\bar{\delta}^{(a)}$ defined in (2.6). The three contributions depicted in figure 2 are described below.

JHEP06(2023)089

- *Perturbation theory* is given by

$$\rho_{\Pi}(s,\tilde{s}) = \frac{m_+^2 N_c m_q}{2\pi^2} \frac{s-(m_b-m_q)^2}{s+m_q^2-m_b^2} \lambda^{\frac{1}{2}} \delta(\tilde{s}-s)\,, \tag{3.5}$$

  with the anticipated $\mathcal{O}(m_q)$-suppression. This term is negligible and it is noted that there is no m_b-type term.

- *The $\langle \bar{q}q \rangle$ condensate* evaluates to

$$\langle \bar{B}|\bar{q}q|\bar{B}\rangle = -\frac{4m_+^2}{Z_B^2} e^{\frac{2(m_B^2-m_b^2)}{M^2}} \langle 0|\bar{q}q|0\rangle \left(m_b^2 + \mathcal{O}(m_q m_b, m_q^2)\right), \tag{3.6}$$

  which is not suppressed by $\mathcal{O}(m_q)$ and thus dominant.

- *The mixed condensate* yields

$$\langle \bar{B}|\bar{q}q|\bar{B}\rangle = -\frac{m_+^2 \langle \bar{q}\sigma s_g g G q\rangle}{Z_B^2} e^{\frac{2(m_B^2-m_b^2)}{M^2}} \left(\left(1-\frac{3m_b^2}{M^2}\right) + \left(\frac{5}{8}+\frac{2m_b^2}{M^2}-\frac{4m_b^4}{M^4}+\ldots\right)\right), \tag{3.7}$$

  which is not suppressed either as it is in the same chirality representation as the quark condensate. The dots correspond to $m_b m_q$ and m_q^2-terms which are negligibly small as in the condensate case above. The first and second term in round brackets are from the third and fourth diagram in figure 2.

We consider it worthwhile to comment how the lack of m_q-suppression in the condensate contribution arises. Its origin is the propagator $1/(r^2 - m_q^2 + i\epsilon)$ (we work in the $\vec{r} = 0$ frame)

$$r^2 - m_q^2 + i\epsilon = (\sqrt{s} - (\sqrt{\tilde{s}} + m_q - i\epsilon'))(\sqrt{s} - (\sqrt{\tilde{s}} - m_q + i\epsilon'))\,, \tag{3.8}$$

which when cut gives a term of the form $\frac{\sqrt{s}}{m_q}\delta(s - (\sqrt{\tilde{s}} + m_q)^2)$. The $1/m_q$ thus removes the $\mathcal{O}(m_q)$-suppression in the numerator. Numerically perturbation is entirely negligible and this is also the reason for not including the gluon condensate which is expected to be further suppressed $\mathcal{O}(\Lambda_{\rm QCD}^4/M^4)$ as compared to perturbation theory.

3.1.1 Numerics

The basic procedure for the numerics is the same as described in section 2.1.1. However, the choice of scheme is not as important in this case. Any of the schemes, pole, kinetic and $\overline{\rm MS}$ give similar results and indicate stability. The situation is certainly clearer with respect to the m_b-mass itself as the matrix element is $\mathcal{O}(m_b)$ (3.1) and $\Delta m_B|_{m_q}$ itself is $\mathcal{O}(m_b^0)$ whereas $\Delta m_B|_{\rm QED}$ is computed from a non-local correlation function where the m_b-dependence is more difficult to track. Since the perturbative contribution is suppressed, there is no s_0 dependence (there would be at NLO in α_s). Hence we can fix the Borel value M^2 to satisfy the daughter sum rule (2.10), obtaining the following sum rule parameters

$$\{s_0, \hat{M}^2\}_B = \{35.0, 4.0\}\,{\rm GeV}^2\,, \qquad \{s_0, \hat{M}^2\}_D = \{6.0, 0.75\}\,{\rm GeV}^2\,, \tag{3.9}$$

JHEP06(2023)089

and daughter sum rules

$$
\begin{aligned}
\mathrm{U}(s_0, \hat{M}^2 \pm 0.15\,\mathrm{GeV})_{\Delta m_B|_{m_q}} =& 1.00^{+0.03}_{-0.02}\,, \\
U(s_0, \hat{M}^2 \pm 0.05\,\mathrm{GeV})_{\Delta m_D|_{m_q}} =& 1.00^{+0.20}_{-0.12}\,.
\end{aligned}
\tag{3.10}
$$

Using the input parameters in table 2 (with $m_b^{\text{kin}}(1\,\mathrm{GeV}), \bar{m}_c(\bar{m}_c)$), the $f_{B,D}$ sum rule to LO (cf. appendix B.1) and (3.9) we get

$$
\langle \bar{B}|\bar{q}q|\bar{B}\rangle_{\mu=1\,\mathrm{GeV}} = 5.99^{+1.99}_{-1.41}\,\mathrm{GeV}\,, \qquad \langle \bar{D}|\bar{q}q|\bar{D}\rangle_{\mu=\bar{m}_c\,\mathrm{GeV}} = 3.40^{+1.78}_{-1.71}\,\mathrm{GeV}\,, \tag{3.11}
$$

for the matrix elements and

$$
\Delta m_B|_{m_q} = -1.88^{+0.49}_{-0.71}\,\mathrm{MeV}\,, \qquad \Delta m_D|_{m_q} = +2.68^{+1.48}_{-1.38}\,\mathrm{MeV}\,, \tag{3.12}
$$

for the mass differences.

As this is a LO computation the errors are large, primarily coming from M^2 with a small contribution (20%) from the light quark masses. Note that the set value of M^2 is not independent of higher order α_s corrections. For the D-meson especially, the convergence of the sum rule is not good. This is reflected in the mixed condensate contributing a sizeable 20%-uncertainty. On inspection the ratio of $\Delta m_D|_{m_q}$ to $\Delta m_B|_{m_q}$ is noticeably larger than the $\mathrm{SU}(3)_F$ estimates in (3.15). However this is easily within the given errors which are very large due to the poor quality of the leading order sum rule.

3.2 $\mathrm{SU}(3)_F$ estimates of $\langle \bar{H}|\bar{q}q|\bar{H}\rangle$ for $H = B, D$

Alternatively, one may use $\mathrm{SU}(3)_F$ flavour symmetry $\langle B|\bar{q}q|B\rangle \approx \langle B_s|\bar{s}s|B_s\rangle$ to estimate $\langle B|\bar{q}q|B\rangle$ [13]. Following this analysis one may write ($m_{ud} \equiv \frac{1}{2}(m_u + m_d)$)

$$
(2m_{B_s}^2 - m_{B^+}^2 - m_{B^0}^2) = 2(m_s - m_{ud})\langle B|\bar{q}q|B\rangle\,, \tag{3.13}
$$

from which

$$
\langle B|\bar{q}q|B\rangle \approx \frac{m_{B_s}^2 - m_B^2}{(m_s - m_{ud})}\,, \tag{3.14}
$$

follows. Employing the input from the PDG [35] this leads to[9]

$$
\Delta m_B|_{m_q} = -2.37^{+0.35}_{-0.43} \pm 20\%_{SU_3}\,\mathrm{MeV}\,, \qquad \Delta m_D|_{m_q} = +2.81^{+0.51}_{-0.41} \pm 20\%_{SU_3}\,\mathrm{MeV}\,. \tag{3.15}
$$

We have added a characteristic 20% $\mathrm{SU}(3)_F$-violation due to the use of the $\langle B|\bar{q}q|B\rangle \approx \langle B_s|\bar{s}s|B_s\rangle$. The result are well compatible with (3.12) and we shall not use them any further. Note that in the heavy quark limit we have $\Delta m_B|_{m_q} = -\Delta m_D|_{m_q}$ since the c and b are up and down quark types respectively. This heavy quark limit relation holds reasonably as already observed in [13] (with slightly different input).

[9]Or taking the $\eta \to 3\pi$ analysis [36], which in this case makes a difference, results in

$$
\Delta m_B|_{m_q} = -2.54^{+0.17}_{-0.18} \pm 20\%_{SU_3}\,\mathrm{MeV}\,, \quad \Delta m_D|_{m_q} = +3.01^{+0.21}_{-0.20} \pm 20\%_{SU_3}\,\mathrm{MeV}\,,
$$

a more precise result.

3.3 Soft Goldstone estimate of $\langle L|\bar{q}q|L\rangle$ for $L = \pi, K$

The matrix elements $\langle L|\bar{q}q|L\rangle$ where $L = \pi, K$ is a pseudo-Goldstone boson may be estimated using soft-pion techniques which in this case lead to the famous GMOR-relation [37]. Concretely [38]

$$m^2_{\pi^{+,0}} = (m_u + m_d)B_0\,, \qquad m^2_{K^+} = (m_u + m_s)B_0\,, \qquad m^2_{K^0} = (m_d + m_s)B_0\,, \tag{3.16}$$

which are to first order in the quark masses, with no QED corrections and the constant is $B_0 = -\frac{2\langle\bar{q}q\rangle}{f_\pi^2} \approx 2.26\,\text{GeV}$ at $\mu = 2\,\text{GeV}$. We see that for the pions there is no difference to linear order which is a consequence of isospin [11]. The pion mass splitting is a $\Delta I = 2$ isospin effect since the relevant matrix element has two pion states where the quark masses themselves are of $\Delta I = 1$. Hence it takes at least two powers of the quark mass difference. Fortunately, the latter follows in a straightforward manner from chiral perturbation theory and one obtains to LO

$$\begin{aligned}
\Delta m_K|_{m_q} &= \frac{m_u - m_d}{m_s - m_{ud}} \frac{m_K^2 - m_\pi^2}{2m_K} = \frac{m_u - m_d}{2m_{ud}} \frac{m_\pi^2}{2m_K} = -\,6.74^{+0.98}_{-1.21}\,\text{MeV}\,, \\
\Delta m_\pi|_{m_q} &= \frac{1}{16} \frac{m_d - m_u}{m_s - m_{ud}} \frac{m_d - m_u}{m_{ud}} m_\pi \qquad\qquad = +\,0.16^{+0.06}_{-0.05}\,\text{MeV}\,,
\end{aligned} \tag{3.17}$$

using the values from the PDG [35]. As expected the pion contribution is rather small as a result of being second order in the quark mass difference. It is noteworthy that one obtains $\Delta m_K|_{m_q} \approx -5.7\,\text{MeV}$ when using (3.16) directly which can be seen as a $\text{SU}(3)_F$ correction which is well covered by the quoted uncertainty.

4 Final overview and conclusions

In this paper we have computed the mass difference of the charged and neutral B-, D- and K-mesons. The results, which originate from electromagnetic and quark mass effects, are summarised and contrasted with experimental values in table 1. The electromagnetic contribution is computed from the second order formula (1.3) in section 2 and may be regarded as the core part of this paper. $\Delta m_\pi|_{\text{QED}}$ is taken from a soft-pion theorem (cf. appendix D.2) for completeness and comparison. Quark mass effects are obtained from the Feynman-Hellman formula (1.7) and its corresponding matrix element is computed in section 3.1 for the B and the D respectively whereas for the K and the π a soft theorem turns out to be more reliable.

The results obtained are consistent with the current experimental values. The uncertainties are above 20% and indeed more cannot be expected from a double dispersion sum rule at leading order in the strong coupling constant. Experimental uncertainties are one or two orders of magnitude lower.

The values in table 1 deserves some comments as they are not easily guessed by rules of thumb by a practitioner in non-perturbative QCD. The parametric estimate of $\Delta m_H|_{\text{QED}} = c\,Q_H^{\text{eff}} \frac{\alpha}{\pi} \Lambda_{\text{QCD}}$ with $\Lambda_{\text{QCD}} = 200\,\text{MeV}$ and $Q_D^{\text{eff}} = 2Q_{B,K}^{\text{eff}} = 2/3$, leads to $c \approx$ 10-20 which is a rather large number. To put this into perspective, one should keep in

H	$\Delta m_H\vert_{\text{QED}}$	$\Delta m_H\vert_{m_q}$	Δm_H	$\Delta m_H\vert_{\text{PDG[35]}}$
B	$+1.58(24)$ MeV	$-1.88(60)$ MeV ^{a}	$-0.30(65)$ MeV	$-0.32(5)$ MeV
D	$+2.25(70)$ MeV	$+2.7(1.4)$ MeV ^{a}	$+4.9(1.6)$ MeV	$+4.822(15)$ MeV
K	$+1.85(54)$ MeV	*$-6.7(1.1)$ MeV* ^{b}	$-4.9(1.2)$ MeV	$-3.934(20)$ MeV
π	*$+4.8(1.2)$ MeV* ^{c}	*$+0.16(5)$ MeV* ^{b}	$+5.0(1.2)$ MeV	$+4.5936(5)$ MeV

Table 1. Our values of Δm_H due to the electromagnetic mass difference and the quark masses compared to the PDG values. The entries marked with ^{a} are obtained from the $\langle H|\bar{q}q|H\rangle$ matrix element in conjunction with the Feynman-Hellman theorem (valid to LO in m_q). The values in italic should *not* be regarded as predictions of this work. E.g. ^{b}derived from the soft theorem for (pseudo-) Goldstone bosons (cf. appendix 3.3) and ^{c}results from soft theorem in conjunction with the Weinberg sum rules (cf. appendix D.2). It is noteworthy that $\Delta m_\pi|_{m_q} = \mathcal{O}((m_u - m_d)^2)$ which explains its smallness. For comparison some lattice values $\Delta m_D = 5.47(53)\,\text{MeV}$ and $\Delta m_K = -4.07(15)(15)\,\text{MeV}$ [4] and $\Delta m_D = 4.68(10)(13)\,\text{MeV}$ [3] which are of course more precise as the lattice is suited for mass determination, even in the presence of QED, and due to the full inclusion of QCD.

mind that these kind of estimates are not straightforward as the mass difference is obtained from a non-local (long distance) correlation function (1.3). The scale for the quark mass effect is of course set me $m_u - m_d \approx 2.5\,\text{MeV}$ and its sign depends on whether the non $q = u, d$ quark is of the up (charm) or down (beauty, strange) type quark. The cancellation to almost an order of magnitude of the electric and the quark mass contribution for the B-meson is remarkable, leading to an inflated uncertainty in Δm_B.

Indeed numerically the uncertainties are comparable to previous studies. However the main aim of this paper was to show that it is possible to understand the isospin mass difference from QCD sum rules, that is to obtain values compatible with experiment. The sum rule computation could be improved by including radiative corrections in the strong coupling constant which would be a formidable task. Perhaps more interestingly, the formalism developed in this paper could be applied to baryons to obtain the proton-neutron mass difference for instance.

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A Variants of quark-hadron duality

In this appendix we elaborate on variations of quark-hadron duality. This is best explained by example. Consider the axial correlator in connection with the K

$$\Pi_{\alpha\beta} = i\int d^4x e^{ipx}\langle 0|TA^\dagger_\alpha(x)A_\beta(0)|0\rangle = p_\alpha p_\beta \Pi(p^2) + g_{\alpha\beta}\hat{\Pi}(p^2)\,, \tag{A.1}$$

with A_β defined in (2.13). The Kaon appears in the first structure

$$\Pi(p^2) = \frac{f_K^2}{m_K^2 - p^2} + \dots \,, \tag{A.2}$$

where the dots stand for higher states as usual. QCD sum rules consists of two steps. Firstly the observation that

$$\Pi(p^2) \approx \Pi(p^2)_{\mathrm{pQCD}} \,, \tag{A.3}$$

for some p^2 outside the physical region (could be $p^2 < 0$), where pQCD stands for perturbative QCD with OPE improvements. In a second step one rewrites eq. (A.3) as a dispersion relation followed by a Borel transform under which $(s-p^2)^{-1} \to \exp(-s/M^2)$ (M^2 is the Borel parameter) which results in

$$\int_0^\infty e^{-s/M^2} \rho(s) \approx \int_0^\infty e^{-s/M^2} \rho_{\mathrm{pQCD}}(s) \,, \tag{A.4}$$

with $\rho(s) = \frac{1}{2\pi i} \mathrm{disc}_s \Pi(s) = f_K^2 \delta(s - m_K^2) + \dots$ and the pQCD part is defined analogously. The one assumption is then that this integral can be broken up as follows

$$\int_0^{s_0} e^{-s/M^2} \rho(s) \approx \int_0^{s_0} e^{-s/M^2} \rho_{\mathrm{pQCD}}(s) \,, \tag{A.5}$$

and (A.5) is sometimes referred to as semi-global quark hadron duality [39]. One way to determine s_0 is to impose the daughter sum rule (2.1) and then for consistency with the duality assumption s_0 ought to be somewhere between $(m_K + 2m_\pi)^2$ and $(m_K + 4m_\pi)^2$.

We want to briefly contemplate for which types of weight functions $\omega(s)$ (A.5)

$$\int_0^{s_0} e^{-s/M^2} \rho(s)\omega(s) \approx \int_0^{s_0} e^{-s/M^2} \rho_{\mathrm{pQCD}}(s)\omega(s) \,, \tag{A.6}$$

with corresponding (2.1)

$$m_B^2 = \int_{\mathrm{cut}}^{s_0} e^{-s/M^2} \rho_{\mathrm{pQCD}}(s)\omega(s)\, s\, ds / \Big(\int_{\mathrm{cut}}^{s_0} e^{-s/M^2} \rho_{\mathrm{pQCD}}(s)\omega(s) ds \Big) \,, \tag{A.7}$$

can hold. The crucial point is to be able to justify the analogue of eq. (A.3).

A.1 Weight function $\omega(s) = s$

We might start by rewriting the $p_\alpha p_\beta$-part in (A.1) as follows

$$p_\alpha p_\beta \Pi(p^2) = \frac{p_\alpha p_\beta}{p^2} (p^2 \Pi(p^2)) \,. \tag{A.8}$$

For the pQCD part one may directly write $\rho_{\mathrm{pQCD}}(s) \to s\rho_{\mathrm{pQCD}}(s)$ since p^2 does not lead to new singularities. Using (A.2), the QCD part can be written as

$$(p^2 \Pi(p^2)) = p^2 \frac{f_K^2}{m_K^2 - p^2} + \dots = -f_K^2 + m_K^2 \frac{f_K^2}{m_K^2 - p^2} + \dots \,, \tag{A.9}$$

where $-f_K^2$ is a constant that will disappear under Borel transformation and thus $\rho(s) \to s\rho(s)$ works the very same way. The analogue of (A.3) can be justified in this case by replacing $A^\dagger_\alpha(x) \to -\partial^2 A^\dagger_\alpha(x)$ (A.1).[10] Weight functions of polynomials are generally referred to as moments and are familiar to the community e.g. moments in $b \to c\ell\nu$ for example [40]. It is quite clear that one can not take arbitrarily high powers of moments as then duality will be challenged. Global duality, which is equivalent to a dispersion relation, is only strictly valid for the $n = 0$ case and deviating in higher n is therefore not safe.

A.2 Weight function $\omega(s) = \frac{1}{s-\eta}$

Choosing a weight function

$$\omega(s) = \frac{1}{s-\eta}\,, \tag{A.10}$$

is equivalent to working with a subtracted dispersion relation fo the form

$$\frac{\Pi(p^2) - \Pi(\eta)}{p^2 - \eta} = \int \frac{ds\rho(s)}{(s-p^2)(s-\eta)} + c\,, \tag{A.11}$$

where $c = -\int ds\rho^A(s)/(s(s-\eta)) + \Pi^{'}(\eta)$ is a subtraction constant such that the limit $p^2 \to 0$ comes out correctly. The constant c is though not important in the end as it vanishes under Borel transformation. The question of whether one can use (A.10) then turns into the question whether the left hand side can be computed reliably.

In our application to Kaons we have chosen $\eta = 0$ which is close but still below the Kaon resonance. We have checked that for the f_K sum rule with $s_0 = 0.7\,\mathrm{GeV}^2$ the agreement is reasonable and this serves at least as a partial justification of the procedure in section 2.2.

B Numerical input

The numerical QCD input is summarised in table 2 and below we give the numerical values of the decay constant from sum rule which are the effective LSZ factors.

B.1 Decay constants f_B, f_D and f_K

The extraction of both the QED mass shifts and the linear quark mass corrections, require values for the decay constants f_B, f_D and f_K. Note that, for consistency with the rest of this paper these are evaluated at LO in QCD. The LO expressions for the pseudoscalar (B, D) and axial (K) correlators are well known (e.g. [44, 45]). The following values

$$\begin{aligned} f_B &= 0.157\,\mathrm{GeV}\,, & \{s_0, M^2\} &= \{33.5, 6.0\}\,\mathrm{GeV}^2\,, \\ f_D &= 0.158\,\mathrm{GeV}\,, & \{s_0, M^2\} &= \{5.7, 2.0\}\ \ \mathrm{GeV}^2\,, \\ f_K &= 0.147\,\mathrm{GeV}\,, & \{s_0, M^2\} &= \{1.1, 1.5\}\ \ \mathrm{GeV}^2\,, \end{aligned} \tag{B.1}$$

are obtained.

[10]In our case this is not trivial as $A^\dagger_\alpha$ is not QED gauge invariant but it can still be used at LO. In the general case this requires more thought.

JHEP06(2023)089

$J^P = 0^-$ Meson masses [35]					
m_B	m_{B_s}	m_D	m_{D_s}	m_K	m_π
5.280 GeV	5.367 GeV	1.867 GeV	1.968 GeV	0.496 GeV	0.137 GeV
$J^P = 0^-$ Mass Differences [35]					
Δm_B	Δm_D	Δm_K	Δm_π		
$-0.32(5)$ MeV	$+4.822(15)$ MeV	$-3.934(20)$ MeV	$+4.5936(5)$ MeV		
Quark masses [35]					
$\bar{m}_b(m_b)$	$\bar{m}_c(m_c)$	$m_b^{\rm pole}$	$m_c^{\rm pole}$	$m_b^{\rm kin}\vert 1\text{GeV}$	$m_c^{\rm kin}\vert 1\text{GeV}$
$4.18^{+0.03}_{-0.02}$ GeV	1.27(2) GeV	4.78(6) GeV	1.67(7) GeV	4.53(6) GeV	1.13(5)
$\bar{m}_{s\vert 2\text{GeV}}$	$\bar{m}_{d\vert 2\text{GeV}}$	$\bar{m}_{u\vert 2\text{GeV}}$	$\bar{m}_{ud}\vert 2\text{GeV}$	$\frac{\bar{m}_u}{\bar{m}_d}$	$\frac{\bar{m}_s}{\bar{m}_{ud}}$
$93.4^{+8.6}_{-3.4}$ MeV	$4.67^{+0.48}_{-0.17}$ MeV	$2.16^{+0.49}_{-0.26}$ MeV	$3.45^{+0.35}_{-0.15}$ MeV	$0.474^{+0.056}_{-0.074}$	$27.33^{+0.67}_{-0.77}$
Condensates					
$\langle\bar{q}q\rangle_{\vert 2\text{GeV}}$ [41]	$\langle\bar{s}s\rangle_{\vert 2\text{GeV}}$ [42]	m_0^2 [43]	$\langle 0\vert\frac{\alpha}{\pi}G^2\vert 0\rangle$ [26]		
$-(269(2)\text{ MeV})^3$	$1.08(16)\ \langle\bar{q}q\rangle$	$0.8(2)\text{ GeV}^2$	$0.012(4)\text{ GeV}^4$		

Table 2. Summary of input parameters. Note as inputs into the sum rules we use $m_H = m_{H^-}$, as which has a completely negligible impact. The quantity $m_{ud} \equiv \frac{1}{2}(m_u + m_d)$ is the light quark average. The mixed condensate is parameterised as $\langle\bar{q}\sigma s_g g G q\rangle = m_0^2\langle\bar{q}q\rangle$ as is standard in the literature.

C Double cuts, self energies and condensates for $\Delta m_H|_{\rm QED}$

In this appendix we give some more details of the double cuts required for the double dispersion and we present some extra computations: the self energies and condensate contributions to $\Delta m_B|_{\rm QED}$. These are important for stabilising the sum rules but do not affect the actual value of $\Delta m_B|_{\rm QED}$ per se. This is the case since graphs proportional to Q_b^2 are cancelled in the mass difference. The only non-zero graph contributing to the mass shift is the q-q self energy, but it is numerically negligible. We wish to note that in all these graphs explicit gauge independence has been verified to hold after the double-cut is taken.

C.1 Perturbation theory: $b - q$ diagram

This corresponds to diagram 1 (left) of figure 1 where the photon connects the b and q quarks. The required double discontinuity comes from cutting all 4 quarks simultaneously (that is putting them on shell using the Cutkovsky rules). Once cut, the corresponding spectral density is

$$\rho_{\Gamma_{bq}}(s,\tilde{s}) = -\frac{4\pi^3 N_c m_+^2 Q_b Q_q \alpha}{m_B}\int\frac{d^4q\, d^4l}{(2\pi)^8}\delta^+(l^2-m_q^2)\delta^+((p_B-l)^2-m_b^2) \\ \delta^+(q^2-m_q^2)\delta^+((\tilde{p}_B-q)^2-m_b^2)\frac{N}{(q-l)^2}\,, \qquad \text{(C.1)}$$

where N is the numerator trace structure in Feynman gauge and l and q are loop momenta running through the left and right hand side of the diagram respectively. These integrals can be done with the help of the delta functions with the resulting logarithm in (2.7)

JHEP06(2023)089

coming from the angular integration of the denominator $(q-l)^2$. The result (eq. (2.7) in the main text) is numerically dominant. For the sake of clarity let us explain the link to the Cottingham formula (1.3). Comparing (C.1) to the latter one infers that $T_\mu^{(B)\mu}(q)$ corresponds to $\rho_{\Gamma_{bq}}(s,\tilde{s})$, with the $d^4q/(q-l)^2$-part separated off, integrated over the dispersive s, s'-variables as in (2.5).

C.2 Perturbation theory: self energies

As mentioned the self energy graphs of figure 1 (middle-left and middle-right) are not relevant to the mass splitting. The $b-b$ graph cancels once we take the mass difference while the $q-q$ graph is numerically negligible. The procedure for these diagrams is broadly similar to the $b-q$ diagram above except now the photon loop is completely separate of the two B meson states. This introduces a degeneracy between the cuts which forces $\tilde{s}=s$ (see below). That is, once we have taken the discontinuity in s the remaining propagator becomes proportional to $s-\tilde{s}$. The photon d^4q loop factorises and can be evaluated completely in terms of Passarino-Veltman functions. The perturbative b-b self energy graph, after mass renormalisation, takes on the form

$$\rho_{\Gamma_{bb}}(s,\tilde{s}) = \frac{N_c m_+^2 Q_b^2 \alpha}{32\pi^3 m_B} \cdot \lambda^{\frac{1}{2}} \cdot \frac{s-m_-^2}{s+m_+m_-} f^{\mathrm{R}}(m_b^2)\delta(\tilde{s}-s)\,, \tag{C.2}$$

with the renormalised f^{R},[11]

$$f^{\mathrm{R}}(m^2) = f(m^2) + \frac{32\pi^2 m^2}{e^2}\delta Z_m = \begin{cases} 2m^2\left(4+3\ln\frac{\mu^2}{m^2}\right), & \overline{MS} \\ 0, & \text{Pole} \\ 2m^2\left(\frac{16\mu}{3m}+\frac{2\mu^2}{m^2}\right), & \text{Kinetic} \end{cases} \tag{C.3}$$

$$f(m^2) = 4m^2 B_0(m^2,0,m^2) + (d-2)A_0(m^2)\,. \tag{C.4}$$

The functions A_0 and B_0 are the standard Passarino-Veltman functions with (FeynCalc) normalisation $(2\pi\mu)^{2\epsilon}\int \mathrm{d}^dk\,/(i\pi^2)$. Explicitly these are

$$B_0(m^2,0,m^2) = \frac{1}{\hat{\epsilon}} + 2 + \log\left(\frac{\mu^2}{m^2}\right), \qquad A_0(m^2) = m^2\left(\frac{1}{\hat{\epsilon}} + 1 + \log\left(\frac{\mu^2}{m^2}\right)\right)\,, \tag{C.5}$$

with $\frac{1}{\hat{\epsilon}} = \frac{1}{\epsilon} - \gamma_E + \log 4\pi$. The q-q graph can be obtained by replacing $b \to q$ in the result and since it is $\mathcal{O}(m_q^2)$ it is negligible.

C.3 Condensates

The only relevant condensate graph is given in figure 1 (4th diagram). There are two quark propagators $p_B^2 - m_b^2$ and $\tilde{p}_B^2 - m_b^2$ which are both cut giving simple delta functions. With $m_q \to 0$ the density is

$$\rho^{\langle\bar{q}q\rangle}_{\Gamma_{bb}} = -\frac{m_b^2\alpha Q_b^2}{8\pi m_B} m_b\langle\bar{q}q\rangle\delta(s-m_b^2)\delta(\tilde{s}-m_b^2)f^{\mathrm{R}}(m_b^2)\,. \tag{C.6}$$

[11] Note that the vanishing in the pole scheme is clear, by the very definition of the scheme, since we are on-shell after the cuts.

Light quark mass corrections come from Taylor expanding the quark fields, leading to derivatives of δ-functions. It is thus more convenient to directly display the resulting mass shift

$$\Delta m_B|_{\langle \bar{q}q\rangle} = -\frac{m_+^2 \alpha Q_b^2}{8\pi m_B Z_B^2} e^{\frac{2(m_B^2-m_b^2)}{M^2}} \langle \bar{q}q\rangle \Big(m_b - \frac{m_q}{4}(1+\frac{4m_b^2}{M^2})\Big) f^{\mathrm{R}}(m_b^2) \tag{C.7}$$

The $\langle \bar{q}q\rangle$ condensate graph where the photon connects the b and the q-quark is not of short distance type (it leads to $1/m_q^2$ in the propagator) and is therefore omitted. This is similar to the $B \to \gamma$ form factor although in that case the physics is covered by the photon distribution amplitude (e.g. [33]). The same problem afflicts the similar $\langle \bar{q}q\rangle$ $q-q$ graph.

D Some classic results

In this appendix we summarise some classic results which are of use and referred to in the paper.

D.1 Linear quark mass dependence from Feynman-Hellman theorem

In order to derive the Feynman-Hellman theorem it is convenient to use states $\langle \hat{B}(p)|\hat{B}(q)\rangle = (2\pi)^3\delta^{(3)}(\vec{p}-\vec{q})$ normalised in a non-relativistic manner (the translation to the usual states is $|\hat{B}\rangle = |B\rangle/\sqrt{2E_B}$). Taking the derivative of $\langle \hat{B}|H|\hat{B}\rangle$ (using $\partial_{m_q}\langle \hat{B}(p)|\hat{B}(q)\rangle = 0$) one obtains

$$m_q \partial_{m_q} E_B = m_q \langle \hat{B}|\bar{q}q|\hat{B}\rangle \,, \tag{D.1}$$

which is equivalent to

$$m_q \partial_{m_q} 2E_B^2 = 2m_q \langle B|\bar{q}q|B\rangle \,, \tag{D.2}$$

which in turn is consistent with

$$m_B^2|_{m_q} = \sum_q m_q \langle B|\bar{q}q|B\rangle + \mathcal{O}(m_q^2, m_q^2 \ln mq) \,, \tag{D.3}$$

since the momenta are independent of the mass. This is the relation quoted in (1.6) in the main text.

D.2 $\Delta m_\pi|_{\mathrm{QED}}$ from soft theorem and Weinberg sum rules

Using soft-pion techniques it was shown that [2]

$$\Delta m_\pi|_{\mathrm{QED}} = \frac{3\alpha}{8\pi m_\pi f_\pi^2}\int_0^\infty ds s \ln\frac{\mu^2}{s}(\rho_V(s)-\rho_A(s)) + \mathcal{O}(m_\pi^2/m_\rho^2) \,, \tag{D.4}$$

where $\rho_V = f_\rho \delta(s-m_\rho^2) + \ldots$ is the spectral density of the vector triplet current and ρ_A is the analogous quantity for the axial case. The $\ln s$-term originates from integrating over the photon momentum d^4q. We refer the reader to [11] for an improved treatment using chiral perturbation theory. In fact, as is the case for all soft-pion results, eq. (D.4) follows from the LO electromagnetic term in the Lagrangian and can therefore be systematically improved beyond the soft limit to the extent that its low energy constants (i.e. couplings) are known. Using the Weinberg sum rules [46], which are phenomenologically successful, a good estimate was obtained [2]. Taking the equations resulting from the so-called first and second Weinberg sum rule in [47], then

$$f_\rho^2 = f_{a_1}^2 + f_\pi^2 \,, \quad m_\rho^2 f_\rho^2 = m_{a_1}^2 f_{a_1}^2 \,, \tag{D.5}$$

(where the chiral limit $m_q = 0$ is assumed). Moreover, the spectral functions are truncated after the first vector meson resonances ρ and a_1 which can be justified as the chiral symmetry is restored at high energy. Using these in expressions in (D.4) one gets

$$\Delta m_\pi|_{\mathrm{QED}} = \frac{3\alpha}{8\pi} \frac{m_\rho^2 f_\rho^2}{m_\pi^2 f_\pi^2} m_\pi \ln \frac{f_\rho^2}{f_\rho^2 - f_\pi^2} \approx 4.8\,\mathrm{MeV} \,, \tag{D.6}$$

for $f_\pi = 131\,\mathrm{MeV}$, $m_\rho = 0.77\,\mathrm{MeV}$ [35] and $f_\rho = 215\,\mathrm{MeV}$ [48]. Since the quark mass effect is small $\mathcal{O}((m_u - m_d)^2)$ (3.17), one has $\Delta m_\pi \approx \Delta m_\pi|_{\mathrm{QED}}$ which is rather close to the experimental value $\Delta m_\pi = +4.5936(5)$ MeV [35]. Clearly (D.6) is a crude approximation as more detailed analyses [11, 49] including finite width effects yields a result which is ca $+1.2\,\mathrm{MeV}$ larger [49]. We therefore assign an uncertainty of this amount to $\Delta m_\pi|_{\mathrm{QED}}$ in table 1.

It is also worthwhile to mention two other interesting aspects in conjunction with $\Delta m_\pi|_{\mathrm{QED}}$. First, by using by using QCD inequalities it has been shown that $\Delta m_\pi|_{\mathrm{QED}} \geq 0$ [50] which is of course well satisfied. Second Dashen's theorem [51] states that $\Delta m_\pi^2|_{\mathrm{QED}} - \Delta m_K^2|_{\mathrm{QED}} = \mathcal{O}(\alpha m_s, \alpha m_q \ln m_q)$ as a result of degeneracy in the $\mathrm{SU}(3)_F$ limit $m_s = m_d = m_u$. The corrections seem rather large and are largely kinematic, the larger K mass in the Kaon propagator [52]. Lattice Monte Carlo simulations have settled this matter to large precision [53] (cf. [54] for a review).

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