### New contributions to heavy quark sum rules

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**Abstract.** We analyze new contributions to the theoretical input in heavy quark sum rules and we show that the general theory of singularities of perturbation theory amplitudes yields the method to handle these specific features. In particular we study the inclusion of heavy quark radiation by light quarks at  $\mathcal{O}(\alpha_s^2)$  and of non-symmetric correlators at  $\mathcal{O}(\alpha_s^3)$ . Closely related with this is that we also propose a solution to the construction of moments of the spectral densities at  $\mathcal{O}(\alpha_s^3)$  where the presence of massless contributions invalidates the standard approach. We circumvent this problem through a new definition of the moments, providing an infrared safe and consistent procedure.

#### 1 Introduction

Sum rules analyses have extensively exploited the relation between the correlator of the quark electromagnetic currents and the cross section of  $e^+e^- \rightarrow$  hadrons under the assumption of quark–hadron duality, to extract fundamental information of hadron systems. The two-point function containing the QCD dynamics of the produced quarks is built from the sum of the electromagnetic vector currents associated to each flavor:

$$\Pi_{\text{had}}^{\mu\nu}(p) = i \int d^4x e^{ipx} 
\times \sum_{q,q'} e_q e_{q'} \langle 0 | T(\overline{q}(x)\gamma^{\mu}q(x)) (\overline{q'}(0)\gamma^{\nu}q'(0)) | 0 \rangle 
= (-g^{\mu\nu}p^2 + p^{\mu}p^{\nu}) \Pi_{\text{had}}(p^2),$$
(1)

where q and q' stand for heavy or light quarks, indistinctly, with electric charges  $e_q$  and  $e_{q'}$ . Here we find two types of correlators: the symmetric ones, both electromagnetic currents corresponding to the same flavor, and nonsymmetric correlators, where  $q \neq q'$ . Strictly, the latter are needed to fully describe the electromagnetic production of hadrons, even in the case where a definite flavor type of hadrons is isolated in the final state. Sum rules analyses applied to heavy quark production are written down in terms of the symmetric correlator built from the vector current  $j_Q^{\mu}(x) = e_Q \overline{Q}(x) \gamma^{\mu} Q(x)$  of the heavy quark Q, and the effects of the non-symmetric correlators are never considered. The reason is that they begin to contribute beyond  $\mathcal{O}(\alpha_s^2)$  in QCD perturbation theory (see Fig. 1a), which means one order beyond the actual knowledge of the (symmetric) heavy quark correlator  $\Pi_{O\overline{O}}$ . The study of such new effects in  $Q\overline{Q}$  production will be mandatory if  $\mathcal{O}(\alpha_s^3)$  accuracy is reached in the future. However, already at  $\mathcal{O}(\alpha_s^2)$  the production of heavy quarks  $Q\overline{Q}$  receives contributions which have not been accounted for in the theoretical input of heavy quark sum rules either. These arise from heavy quark discontinuities of symmetric correlators built from quarks such that  $m_q < m_Q$ , as the cut shown in Fig. 1b, representing the production of heavy hadrons radiated off a pair of lighter quarks.

Finally, Groote and Pivovarov have recently pointed out [1,2] that, at  $\mathcal{O}(\alpha_s^3)$ , a three-gluon intermediate state (see Fig. 2) contributes to the  $\Pi_{Q\overline{Q}}$  correlator. As these authors have shown, this massless intermediate state invalidates the usual definition of the moments  $\mathcal{M}_n$ ,

$$\mathcal{M}_n = \frac{1}{n!} \left( \frac{\mathrm{d}}{\mathrm{d}p^2} \right)^n \Pi_{Q\overline{Q}}(p^2) \Big|_{p^2 = 0}, \tag{2}$$

for  $n \geq 4$ , when they become singular. Consequently the use of heavy quark sum rules at  $\mathcal{O}(\alpha_s^3)$  is debatable.

All the features we have just quoted arise as a consequence of the interplay between the implementation of quark–hadron duality and the proper definition of the observables in the case of heavy quarks QCD sum rules. The correlation between the perturbative input and the observable information on the experimental side requires a careful matching that cannot be fully achieved. Accordingly the introduced uncertainties should be estimated and included in the errors of the parameters determined through this method.

Here we discuss the aspects pointed out above and their consequences in the methodology of extracting information from QCD sum rules. The aim of this work is to provide a consistent procedure to implement the perturbative input on the theoretical side of the heavy quark sum rules. Our proposal relies on a careful application of the general theory of singularities of perturbation theory. The crucial point will be to isolate all the cuts related to  $Q\overline{Q}$  production from the general vector two-point function

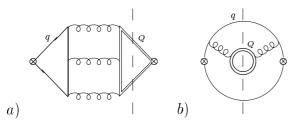


Fig. 1a,b. Examples of perturbative non-heavy quark current correlators at  $\mathcal{O}(\alpha_s^3)$  a and  $\mathcal{O}(\alpha_s^2)$  b that contribute to the production of  $Q\overline{Q}$  states

(1) in order to construct a modified correlator containing only contributions to heavy quark production.

In Sect. 2 we recall the theory of singularities of perturbative amplitudes. The relation between the phenomenological and the theoretical input in the QCD sum rules is discussed in Sect. 3. Hence Sects. 4 and 5 collect the implementation of our proposal to include heavy quark radiation off light quarks and to exclude massless singularities, respectively. We will comment on the uncertainties related with our method too. In Sect. 6 we emphasize our conclusions.

### 2 Analyticity of $\Pi_{\mathrm{had}}(s)$

As is well known two-point functions are analytic except for singularities at simple poles or branch cuts, the latter originating from normal thresholds of production of internal on-shell states. Assuming that the absorptive part of  $\Pi_{\text{had}}(p^2)$  starts at some point  $s_0$ , vanishing below this point, the correlator satisfies the dispersion relation [3]:

$$\widehat{\Pi}_{\text{had}}(p^2) \doteq \Pi_{\text{had}}(p^2) - \Pi_{\text{had}}(0) = \frac{p^2}{\pi} \int_{s_0}^{\infty} \frac{\mathrm{d}s}{s} \frac{\text{Im}\Pi_{\text{had}}(s)}{s - p^2 - i\epsilon}.$$
(3)

The absorptive part  ${\rm Im} \Pi_{\rm had}(s)$  is a physical observable, as it is proportional to the total hadron production cross section by a vector current  $J^\mu = \sum_q j_q^\mu$ . QCD being the underlying theory of strong interactions, the quark–hadron duality hypothesis allows us to identify, inclusively, the states in terms of observable hadrons with the partonic intermediate states. Hence the optical theorem tells us that the total absorptive part is the sum of the absorptive parts corresponding to different intermediate partonic states:

$$\operatorname{Im} \Pi_{\text{had}}(s) = -\frac{1}{6s} \int \sum_{n} dR_{n} \langle 0|J^{\mu}|n\rangle \langle n|J_{\mu}^{\dagger}|0\rangle$$
$$= \sum_{n} \operatorname{Im} \Pi_{n}(s), \tag{4}$$

where the phase space integration has been explicitly stated<sup>2</sup>. A similar separation between contributions of different final hadron states in the perturbative evaluation of the two-point correlator, (1), would allow us to keep only the desired heavy quark cuts in the symmetric and non-symmetric correlators. Although Cutkosky rules provide a method to isolate cuts corresponding to different intermediate states at the perturbative level, some care is needed in their application.

The study of the analytic properties of perturbation theory amplitudes shows that their singularities are isolated and, therefore, we can discuss each singularity of a perturbative amplitude by itself [4]. As a consequence, any one-variable dependent amplitude F(z) satisfies a dispersion relation from Cauchy's theorem given by<sup>3</sup>

$$F(z) = \frac{1}{2\pi i} \oint dz' \frac{F(z')}{z' - z} = \sum_{n} \int_{z_n}^{\infty} \frac{dz'}{2\pi i} \frac{[F(z')]_n}{z' - z}, \quad (5)$$

where  $[F(z)]_n$  is the discontinuity across a branch cut which starts at the point  $z_n$  and is associated to a definite intermediate state. For the general two-point function in (1), which depends on the total momentum squared  $p^2$ , we would have

$$\widehat{\Pi}_{\text{had}}(p^2) = \sum_{n} \frac{p^2}{2\pi i} \int_{s_n}^{\infty} \frac{\mathrm{d}s}{s} \frac{[\Pi(s)]_n}{s - p^2 - i\epsilon},\tag{6}$$

where now  $[\Pi(s)]_n$  provides the sum of all the cut diagrams associated to a definite intermediate state labelled  $n \ (n = q\bar{q}, q'\bar{q}', ggg, q\bar{q}q'\bar{q}', \ldots)$ . In the perturbative calculation, every discontinuity contributing to  $[\Pi(s)]_n$  can be associated to a "reduced" Feynman diagram obtained by contracting internal off-shell propagators to a point and leaving internal on-shell lines untouched. Its contribution is written down following the Cutkosky rules for the graph. However the discontinuity across a specified cut in a single diagram does not need to be a pure real function in the physical region. Hence the separation between the imaginary parts coming from different final states, as stated in (4), does not seem to apply for individual diagrams. But from (4) and (6) we can conclude that  $[\Pi(s)]_n = 2i \text{Im} \Pi_n(s)$ , meaning that only the sum of all cuts corresponding to a defined intermediate state provides the physical observable, i.e.  $\text{Im}\Pi_n(s)$ . Evidently, this holds at any perturbative order in  $\alpha_s$ , and gives a prescription to isolate contributions to different quark intermediate states in the hadron two-point function. This assertion might seem obvious but it is not: A  $Q\overline{Q}$  cut on the righthand fermion loop in Fig. 2a does not provide, by itself, a pure real contribution. Only when both QQ cuts, on the left-hand and right-hand fermion loops of Fig. 2a, are added we get a term contributing to the physical observable  $\operatorname{Im} \Pi_{n=Q\overline{Q}}$ .

 $<sup>^1</sup>$  Sometimes the Adler function defined by  $\partial \Pi(p^2)/\partial \ln p^2,$  to get rid of the subtraction constant, is used. The choice of the regularization prescription is not relevant for our discussion here

We use  $dR_n = (2\pi)^4 \delta^4 \left(q - \sum_{i=1}^n p_i\right) \prod_{i=1}^n dp_i$ , where q is the current four-momentum and  $dp_i = d^3p_i/((2\pi)^3 2E_i)$ . The -1/(6s) factor in (4) originates from  $\Pi_{\text{had}} = -g_{\mu\nu}\Pi_{\text{had}}^{\mu\nu}/(3s)$  and the (1/2) factor from the unitarity relation

<sup>&</sup>lt;sup>3</sup> This expression also gives the residue  $R_i$  of a pole at  $z = z_i$  if we interpret the discontinuity as  $[F(z)]_n = 2\pi i R_i \delta(z - z_i)$ 

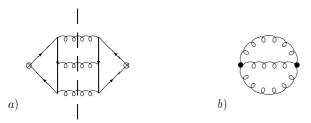


Fig. 2. a  $\mathcal{O}(\alpha_s^3)$  diagram contributing to the vacuum polarization function of the heavy quark current (the vertical dashed line indicates the massless cut). b "Effective" diagram obtained by integrating out the fermion loops. It also has the topological structure of the "reduced" diagram that determines the massless cut singularity

This last example also shows that some subsets of discontinuities of the same intermediate state give already real functions prior to the summation of all contributions at a fixed perturbative order. This is the case for the set of cuts coming from a symmetric correlator, and for the set arising from a non-symmetric correlator with currents  $j_q^{\mu}, j_{q'}^{\mu}$  together with its conjugate. This is easily seen if we rewrite the absorptive part corresponding to the state n, Im $\Pi_n$ , as a sum of terms arising from symmetric and from non-symmetric correlators:

$$\operatorname{Im} \Pi_n(s) = -\frac{1}{6s} \int dR_n \left[ \sum_q \langle 0|j_q^{\mu}|n\rangle \langle n|j_{q,\mu}^{\dagger}|0\rangle \right]$$
 (7)

$$+ \sum_{m_q < m_{q'}} \left( \langle 0 | j_q^\mu | n \rangle \langle n | j_{q',\mu}^\dagger | 0 \rangle + \langle 0 | j_{q'}^\mu | n \rangle \langle n | j_{q,\mu}^\dagger | 0 \rangle \right) \right].$$

The first term in the r.h.s. of (7) represents the absorptive contribution from symmetric correlators, and the perturbative expansion of each one, following Cutkosky rules, is clearly real. In the case of interest<sup>4</sup>,  $n \equiv [Q\overline{Q}]$ , this term contains the usual heavy quark spectral density built from heavy quark currents,  $\Pi_{Q\overline{Q}}$ , and  $[Q\overline{Q}]$  production through light quark currents correlators. The second and third terms in (7) are conjugate to each other, so their sum also gives a pure real number. In terms of diagrams, this means that to extract the desired absorptive part from non-symmetric correlators we need to add to the cut of a diagram the corresponding one in the conjugated diagram (see Fig. 1a; the discontinuity obtained from the same diagram with quark q and quark Q lines interchanged should be added to get a real contribution).

# 3 Phenomenology versus theoretical input in heavy quark sum rules

The analysis above shows that clear control can be enforced on the perturbative side of the sum rules in order to include or exclude specific contributions. However while there is no doubt about the observable that provides  $\text{Im} \Pi_{\text{had}} \propto \sigma(e^+e^- \to \text{hadrons})$  when an exclusive hadron sector (like, for example, heavy quark production) is specified, it is clear that the matching between the perturbative and the phenomenological side includes uncertainties related with the content and definition of the final state.

Heavy quark sum rules [5] have been successful in providing information on the heavy quark parameters. In short they make use of global quark–hadron duality which translates into the ansatz on the vector correlator  $\Pi_{[Q\overline{Q}]}(s)$ :

$$\int_{s_0}^{\infty} ds \frac{\operatorname{Im} \Pi_{[Q\overline{Q}]}^{\operatorname{phen}}(s)}{s^n} \simeq \int_{AM^2}^{\infty} ds \frac{\operatorname{Im} \Pi_{[Q\overline{Q}]}^{\operatorname{pert}}(s)}{s^n} + \cdots, \quad (8)$$

where  ${\rm Im} \Pi^{\rm phen}_{[Q\overline{Q}]}(s)$  on the l.h.s. gives the phenomenological information on heavy quark production and it is related with the cross section of vector current production of hadrons containing Q-flavored states. On the r.h.s. Im  $\Pi^{\rm pert}_{[Q\overline{Q}]}(s)$  is the QCD perturbative contribution to the correlator, and in the lower limit of integration M is usually taken as the pole mass of the heavy quark. Finally the dots on the r.h.s. are short for non-perturbative (the gluon condensate essentially) contributions and possible Coulomblike bound states coming from non-relativistic resummations in  $\Pi^{\rm pert}_{[Q\overline{Q}]}$  below threshold. These last two features are not relevant for the discussion of this paper and have to be implemented on our results without modification.

To a definite perturbative order in  $\alpha_s$ ,  $\text{Im}\Pi^{\text{pert}}_{[Q\overline{Q}]}(s)$  includes all the absorptive contributions to the correlator that provide  $[Q\overline{Q}]$  production. Notice that this is not the same as the absorptive  $Q\overline{Q}$  contribution of the heavy quark current correlator  $\Pi_{O\overline{O}}$ , as is usually assumed. The total experimental cross section  $\sigma(e^+e^- \to \text{hadrons})$  can be split into two disjoint quantities: the cross section for producing hadrons with Q-flavored states, and the production of hadrons with no Q-flavored components. If the experimental set up was accurate enough to classify events into one of these two clusters, the first class would be the required ingredient for the phenomenological part of the heavy quark sum rule. However this separation, implemented on the theoretical side within perturbative QCD, is rather involved. Up to  $\mathcal{O}(\alpha_s^2)$  there has not been any doubt, in the literature, that contributions to this side arise wholly from  $Q\overline{Q}$  cuts in the heavy quark correlator  $\Pi_{Q\overline{Q}}$ . The physical picture behind this assertion relies on the assumption of factorization between hard and soft regions in the quark production process and subsequent hadronization. The hard region described with perturbative QCD entails the production of a pair of heavy quarks, and the soft part of the interaction is responsible for the observed final hadron content. Although possible, annihilation of the partonic state QQ due to the latter interaction is very unlikely, as jets arising from the short distance interaction fly apart before long distance effects become essential. Consequently, each jet hadronizes to a content of Q-flavored states with unit probability. As local duality is implicitly invoked, this picture is assumed to hold

<sup>&</sup>lt;sup>4</sup> Brackets  $[Q\overline{Q}]$  are short for any hadron state containing at least a  $Q\overline{Q}$  pair and, possibly, light quarks and gluons too

at sufficient high energies; hence perturbative corrections to the hard part are successively included through the heavy quark currents correlator. We claim, though, that similar  $Q\overline{Q}$  cuts are present in non-symmetric correlators, starting at  $\mathcal{O}(\alpha_{\rm s}^3)$ , as the one shown in Fig. 1a, where the left-hand part of the cut diagram is a genuine production of  $Q\overline{Q}$  states triggered by virtual light quarks. If the use of heavy quark sum rules up to this order is considered, the inclusion of these terms of the correlator of a heavy and a light quark currents should be taken into account. According to our conclusion in the last section, once the discontinuity provided by Fig. 1a is known, it has to be added to  $\mathrm{Im} \Pi^{\mathrm{pert}}_{[Q\overline{Q}]}(s)$ .

Other extra  $Q\overline{Q}$  cuts, i.e. ones not contained in  $\Pi_{Q\overline{Q}}$ , arise even at  $\mathcal{O}(\alpha_{\mathrm{s}}^2)$  as the diagram of Fig. 1b. In this case the  $Q\overline{Q}$  pair is produced through the splitting of a hard gluon radiated off a pair of light quarks. Whether this cut should be accounted for or not on the theoretical side depends crucially on which the content and the configuration of the reconstructed final state are in the experimental data, as the physical picture outlined above for pure  $Q\overline{Q}$  cuts does not apply so clearly for  $Q\overline{Q}q\overline{q}$  discontinuities. We will come back to this point at the end of Sect. 4. In addition a discussion of other possible contributing cuts should be given. The case of the three-gluon discontinuity is postponed to Sect. 5.

In the following we will discuss, in turn, the inclusion of heavy quark radiation by light quarks and the infrared massless discontinuities noticed by Groote and Pivovarov. We will provide specific solutions along the lines put forward in Sects. 2 and 3.

#### 4 Heavy quark radiation

Starting at  $\mathcal{O}(\alpha_s^2)$ , symmetric correlators built from light quark currents include four fermion cuts with a heavy quark pair radiated off the light quarks as shown in Fig. 1b (two additional diagrams, one with the two gluons attached to the lower light fermion line, and the other with one gluon attached to each light fermion line, should be considered too). The sum of all these four fermion absorptive parts in the three-loop diagrams with massless light quarks currents has been calculated in [6], and can be cast into the following form<sup>5</sup>:

$$12\pi \operatorname{Im} \Pi_{q\overline{q}Q\overline{Q}}(s) = R_{q\overline{q}Q\overline{Q}}$$

$$\equiv N_c \left( \sum_{i=u,d,s} Q_i^2 \right) C_8 \left( \frac{\alpha_s}{\pi} \right)^2 \int_{4M^2}^s \frac{\mathrm{d}s'}{s'} R(s') F(s'/s),$$
(9)

with

$$F(x) = \frac{1}{6} \left\{ (1+x)^2 \ln^2 x + (3+4x+3x^2) \ln x + 5(1-x^2) \right\}$$

$$-4(1+x)^{2}\left[\operatorname{Li}_{2}(-x)+\ln(1+x)\ln x+\frac{\pi^{2}}{12}\right]. (10)$$

The function F(s'/s) gives the rate for the decay of a vector boson of mass  $s^{1/2}$  into a vector boson of mass  $s'^{1/2}$  plus a pair of massless fermions  $(q\bar{q})$ . The spectral density  $R(s) = \beta(3-\beta^2)/2$  (at lowest order) is the normalized cross section for the production of a pair of fermions with unit charge through a vector boson; here  $\beta = (1-4M^2/s)^{1/2}$  is the velocity of the produced heavy quarks. The integral can be solved analytically in this case and the result is found in [6]. Note that the heavy quark pair is created in a color octet state, and the factor

$$C_8 = \frac{1}{N_c} \operatorname{Tr}\left(\frac{\lambda^a}{2} \frac{\lambda^b}{2}\right) \operatorname{Tr}\left(\frac{\lambda^a}{2} \frac{\lambda^b}{2}\right) = \frac{2}{3}$$

retains this color structure. It is interesting to compare the contribution from  $R_{q\overline{q}Q\overline{Q}}$  with the  $\mathcal{O}(\alpha_{\rm s}^2)$  contributions to  $R_{Q\overline{Q}}$  (i.e. to the spectral density of the heavy quark correlator). Note that in the high energy limit there is no difference between the diagram shown in Fig. 1b and the same one with Q and q lines interchanged or with q=Q, both of them being included in  $H_{Q\bar{Q}}$ . Differences arise because the heavy quark currents correlator,  $H_{Q\overline{Q}}$ , also accounts for two heavy quark cuts where the internal (light or heavy) quark loop represents a virtual correction to the electromagnetic current.

We have written (9) in terms of a general R(s) function in the integrand because it allows us to introduce in a straightforward way the final state interactions for the heavy quark pair. In particular, we know that close to threshold the Coulomb interaction between the heavy quark pair dominates the dynamics. Resummation of leading terms  $\sim (\alpha_s/\beta)^n$  becomes mandatory, and gives rise to the well-known Sommerfeld factor multiplying the cross section:

$$R^{\rm thr}(s) = R(s) \times \frac{C\pi\alpha_{\rm s}/\beta}{1 - \exp(-C\pi\alpha_{\rm s}/\beta)}.$$
 (11)

The color factor C appears in the Coulomb QCD potential and its value depends on the relative color state of the quark pair. For singlet states  $C=C_F$ , and the potential is attractive, increasing the cross section at threshold. This is the case of heavy quark production in  $e^+e^-$  collisions. However, in our case the heavy quark pair is produced through the splitting of a gluon. The Coulomb potential becomes repulsive between quarks in a color octet state,  $C=C_F-C_A/2=-1/(2N_c)$ , and the Sommerfeld factor at low velocities then reads

$$\frac{-\pi\alpha_{\rm s}/6\beta}{1-\exp(\pi\alpha_{\rm s}/6\beta)} \stackrel{\beta\to 0}{\Longrightarrow} \frac{\pi\alpha_{\rm s}}{6\beta} e^{-(\pi\alpha_{\rm s})/(6\beta)},$$

causing the cross section to decrease near threshold even faster than  $\beta$ , the phase space velocity in R(s). The production of heavy quarks radiated off massless quarks through a virtual gluon is then very much suppressed in the threshold region. However, as mentioned above, high

 $<sup>^{5}</sup>$  Notice that our definition of  $R_{q\overline{q}Q\overline{Q}}$  differs from the one in [6]

energy quark lines can be considered massless and the contribution from this diagram is numerically equal to the same one with Q and q lines interchanged.

same one with Q and q lines interchanged. The inclusion in  $\text{Im}\Pi^{\text{pert}}_{[Q\overline{Q}]}(s)$  of four-fermion cuts coming from light quark correlators is possible because we have shown in Sect. 2 how to discern and extract these pieces. As discussed before, the procedure depends crucially on the definition of the observable information input in the sum rule, and consistence between the theoretical and phenomenological parts is required. Let us come back to the discussion of Sect. 3. There it was argued why perturbative  $Q\overline{Q}$  cuts are thought to reproduce the phenomenology of two jet events. Notice that, in heavy quark radiation from light quarks, the signature of the event is likely to be a three-jet configuration where one of the jets is generated from a gluon. If heavy flavor components are to be found in this jet, the diagram of Fig. 1b would certainly be needed to account for these events on the theoretical side. However the heavy partons in this jet are not as energetic as in a pure QQ production and, consequently, the proposed factorization between long and short distance effects may no longer apply, allowing for interference between both regimes. In this case we cannot argue that this kind of cut diagrams would result in a final state with Q-flavored hadrons with unit probability, although we may impose kinematical constraints to reduce uncertainties in both the experimental reconstruction of the data and the theoretical cross section of these  $Q\overline{Q}q\overline{q}$  states. This issue is the source of a recent discussion in the literature related with the secondary production of bb through gluon splitting [6,7].

## 5 Massless contribution to heavy quark sum rules

Until presently the evaluation of the perturbative twopoint correlation function  $\Pi^{\text{pert}}(q^2)$  (in this section we will denote the heavy quark currents correlator by  $\Pi(q^2)$ ) has only been carried out completely, with massive quarks, up to  $\mathcal{O}(\alpha_s^2)$  [8] and the sum rules procedure, given by (8), has been termed consistent and effective in its task because the first branch point is set at the massive two-particle threshold. However Groote and Pivovarov have pointed out [1] that at  $\mathcal{O}(\alpha_s^3)$  there is a contribution to the correlator which contains a three-gluon massless intermediate state (see Fig. 2a). Its absorptive part starts at zero energy and, therefore, (8) is no longer correct because on the r.h.s. there is a discontinuity starting at s = 0. Moreover those authors have also warned for the fact that, at this perturbative order, the massless intermediate state invalidates the definition of the moments  $\mathcal{M}_n$  for  $n \geq 4$  because they become singular. Let us recall their reasoning.

The perturbative contribution given by the diagram in Fig. 2a has been calculated at small  $q^2$  ( $q^2 \ll M^2$ ) in [1]. In this limit the quark triangle loop can be integrated out and it ends up in the diagram in Fig. 2b generated by an induced effective current describing the interaction of the vector current with three gluons,

$$J^{\mu} = -\frac{\pi}{180M^4} \left(\frac{\alpha_{\rm s}}{\pi}\right)^{3/2} \left(5\partial_{\nu}\mathcal{O}_{1}^{\mu\nu} + 14\partial_{\nu}\mathcal{O}_{2}^{\mu\nu}\right), \quad (12)$$

with

$$\mathcal{O}_{1}^{\mu\nu} = d_{abc} G_{a}^{\mu\nu} G_{b}^{\alpha\beta} G_{\alpha\beta}^{c},$$

$$\mathcal{O}_{2}^{\mu\nu} = d_{abc} G_{a}^{\mu\alpha} G_{\alpha\beta}^{b} G_{c}^{\beta\nu},$$

$$(13)$$

where  $G_a^{\mu\nu}$  is the gluon strength field tensor. The effective current in the QED case  $(G_a^{\mu\nu} \to F^{\mu\nu}, \alpha_s \to \alpha_{\rm em}, d_{abc} \to 1)$  can easily be identified from the lowest order Euler–Heisenberg Lagrangian (see [2]).

The correlator of the induced current (12) is then evaluated in the configuration space, giving

$$\langle 0|TJ_{\mu}(x)J_{\nu}^{\dagger}(0)|0\rangle \qquad (14)$$

$$= -\frac{34}{2025\pi^{4}M^{8}} \left(\frac{\alpha_{s}}{\pi}\right)^{3} d_{abc}d_{abc} \left(\partial_{\mu}\partial_{\nu} - g_{\mu\nu}\partial^{2}\right) \frac{1}{x^{12}}.$$

In momentum space we need to perform the Fourier transform of (14). Following the differential regularization procedure [9], which works directly in configuration space, the result for the vacuum polarization contribution of the diagram in Fig. 2b at small  $q^2$  reads

$$\Pi_{\mu\nu}(q) = \frac{17}{2916000\pi^2} d_{abc} d_{abc} \left(\frac{\alpha_{\rm s}}{\pi}\right)^3 (q_{\mu}q_{\nu} - q^2 g_{\mu\nu}) \\
\times \left(\frac{q^2}{4M^2}\right)^4 \ln\left(\frac{\mu^2}{-q^2}\right) + \mathcal{O}\left[\left(\frac{q^2}{M^2}\right)^5\right], \quad (15)$$

with  $\mu$  the renormalization point in this scheme, and  $d_{abc}$   $d_{abc} = 40/3$ .

As noticed by Groote and Pivovarov [1], moments associated to the diagram in Fig. 2b are not defined if  $n \geq 4$ . Indeed differentiating (15) four times, at  $q^2 \approx 0$ , we get

$$\frac{1}{4!} \left( \frac{\mathrm{d}}{\mathrm{d}q^2} \right)^4 \Pi(q^2) \bigg|_{q^2 \approx 0} \\
= \frac{17}{218700\pi^2} \left( \frac{\alpha_{\mathrm{s}}}{\pi} \right)^3 \left( \frac{1}{4M^2} \right)^4 \left[ \ln \left( \frac{\mu^2}{-q^2} \right) - \frac{25}{12} \right] \\
+ \mathcal{O} \left[ \frac{q^2}{M^{10}} \right], \tag{16}$$

whose real part clearly diverges if we set  $q^2 = 0$ . Larger n moments are also infrared divergent, and so the authors of [1] conclude that the standard sum rule analysis must limit the accuracy of theoretical calculations for the  $n \geq 4$  moments to the  $\mathcal{O}(\alpha_s^2)$  order of perturbation theory. This is, essentially, the conclusion of [1].

An infrared safe redefinition of the moments, to cure the latter problem, has been provided in [2]; it consists in evaluating the moments at an Euclidean point  $q^2 = -s_{\rm E},\ s_{\rm E} > 0$ , thus avoiding the singular behavior. This solution, as explained by the authors of that reference, is rather ill-conditioned from the phenomenological side though. Nevertheless the flaw in (8) due to the massless threshold still represents a problem because even if, up to  $\mathcal{O}(\alpha_{\rm s}^3)$ , we substitute the dispersion relation by

$$\widehat{\Pi}^{\text{pert}}(q^2) = \frac{q^2}{\pi} \int_{4M^2}^{\infty} \frac{\mathrm{d}s}{s} \frac{\text{Im} \Pi_{Q\overline{Q}}^{\text{pert}}(s)}{s - q^2 - i\epsilon} + \frac{q^2}{\pi} \int_0^{\infty} \frac{\mathrm{d}s}{s} \frac{\text{Im} \Pi_{3g}(s)}{s - q^2 - i\epsilon}$$
(17)

(where  $\text{Im}\Pi_{Q\overline{Q}}^{\text{pert}}(s)$  includes discontinuities starting at  $s=4M^2$ ), the spectral function  $\text{Im}\Pi_{3g}(s)$  associated to the cut in Fig. 2a would hardly be implemented phenomenologically as gluons hadronize to both heavy and light quark pairs. We wish to provide a bypass to recover the balance between the right-hand and left-hand parts of (17). We will now see that if one does not insist on using full vacuum polarization for the sum rule analysis there is a way to overcome this infrared problem.

In the heavy quark correlator the discontinuity across the three-gluon cut gives a contribution to the spectral function that is unequivocally real:

$$\frac{1}{2i} \left[ \Pi(s) \right]_{3g} = \operatorname{Im} \Pi_{3g}(s)$$

$$= -\frac{1}{6s} \int dR_{3g} \langle 0|j^{\mu}|3g \rangle \langle 3g|j^{\dagger}_{\mu}|0 \rangle, \quad (18)$$

from which the dispersive part can be evaluated independently of the  $Q\overline{Q}$  cuts. Accordingly we conclude that we can identify and isolate the troublesome massless cut contribution to the two-point function. Indeed (6) and (18) justify our previous (17).

Let us go back then to (17). All the difficulty with the phenomenological application of the sum rules is now the fact that the contribution from the three-gluon cut is contained in both sides of the equality. This intermediate state hadronizes completely into hadrons with a content of light and/or heavy quarks indistinctly. It is conspicuous that if we could disentangle the heavy quark hadronization,  $3g \to Q\overline{Q}$ , we should include only this piece into the sum rule. Then the singularity at  $q^2 = 0$  would disappear because heavy quarks are produced starting at  $q^2 = 4M^2$ . However there is no way to sort out light and heavy quark production off three gluons and, therefore, if we extract this contribution from the heavy quark sum rules we are introducing an uncertainty in the procedure because we make sure that there is no light quark hadronization but we miss the heavy quark production. It is easy to see that the induced error is small, due to the fact that three gluons hadronize mostly to light hadrons. On one side, in the very high energy region and following perturbative QCD with  $N_F = 4$ , we have only a 1/4 = 25% probability of finding a specified pair of heavy quarks produced. And this is a generous upper limit because when we go down in energy, phase space restrictions severely reduce the counting of heavy quarks. Hence we estimate that excluding the three-gluon cut we introduce a tiny (few percent) error in the sum rules procedure.

Thus we propose an *infrared safe* definition of the moments by the trivial subtraction

$$\widetilde{\Pi}^{\mathrm{pert}}(q^2) \doteq \widehat{\Pi}^{\mathrm{pert}}(q^2) - \frac{q^2}{\pi} \int_0^\infty \frac{\mathrm{d}s}{s} \frac{\mathrm{Im} \Pi_{3g}(s)}{s - q^2 - \mathrm{i}\epsilon}$$

$$= \frac{q^2}{\pi} \int_{4M^2}^{\infty} \frac{\mathrm{d}s}{s} \frac{\mathrm{Im} \Pi_{Q\overline{Q}}^{\mathrm{pert}}(s)}{s - q^2 - \mathrm{i}\epsilon},\tag{19}$$

$$\widetilde{\mathcal{M}}_n \doteq \mathcal{M}_n - \frac{1}{\pi} \int_0^\infty \mathrm{d}s \frac{\mathrm{Im} \Pi_{3g}(s)}{s^{n+1}}.$$
 (20)

Of course (19) and (20) are meaningless unless we give a precise prescription about how to subtract the contribution of the massless cuts represented by  $Im \Pi_{3a}$ . Our previous discussion gives us the tool with which to proceed. Once the full  $\mathcal{O}(\alpha_s^3)$   $\Pi^{\text{pert}}(s)$  is calculated we can extract the imaginary part starting at s = 0 (which should go with a  $\theta(s)$  function) for any value of s. It is clear that the  $\theta(s)$  and  $\theta(s-4M^2)$  terms in the imaginary part of the vacuum polarization function correspond to three-gluon massless and to  $Q\overline{Q}$  cut graphs, respectively, and  $\text{Im}\Pi_{3q}$ and  $\operatorname{Im}_{Q\overline{Q}}^{\operatorname{pert}}$  are easy to distinguish, as (18) prevents the appearance of mixed  $\theta(s) \cdot \theta(s-4M^2)$  terms. Therefore we identify  $\mathrm{Im}\Pi_{3g}$  and we now plug it in the dispersion integral of the right-hand side of (20) and perform such integration. Divergences contained in both this integral and  $\mathcal{M}_n$  as  $q^2 \to 0$  will cancel with each other if the same infrared regularization is employed in the two quantities. The intuitive choice would be a low energy cutoff  $s_0 > 0$ , and (20) would be more precisely written as

$$\widetilde{\mathcal{M}}_{n} \equiv \lim_{s_{0} \to 0^{+}} \left[ \frac{1}{n!} \left( \frac{\mathrm{d}}{\mathrm{d}q^{2}} \right)^{n} \Pi^{\mathrm{pert}}(q^{2}) \right|_{q^{2} = -s_{0}}$$

$$- \frac{1}{\pi} \int_{0}^{\infty} \frac{\mathrm{d}s}{s} \frac{\mathrm{Im} \Pi_{3g}(s)}{(s + s_{0})^{n}} \right], \tag{21}$$

where a vanishing term in the  $s_0 \to 0^+$  limit has been omitted.

The evaluation of the  $\mathcal{M}_n$  moments at  $q^2 = 0 < 4M^2$  made sense because, up to  $\mathcal{O}(\alpha_s^2)$ , this point, being far away from the heavy quark production threshold, is unphysical and the moments are well defined through an analytic continuation from the high energy region. However note that the absorptive three-gluon contribution starts at  $q^2 = 0$  and perturbative QCD becomes unreliable. This introduces a further new difficulty in evaluating  $\mathcal{M}_n$  moments at  $q^2 = 0$ , as we reach the physical non-perturbative region. Our definition of the moments,  $\widetilde{\mathcal{M}}_n$  in (20), skips this problem by fully eliminating the massless terms and, therefore, the final heavy quark sum rule will only involve physics at  $q^2 > 4M^2$ , apart from possible bound states.

The general rule given above is valid for all orders of perturbation theory, but it strongly relies on our ability to extract the massless absorptive part from the full result of  $\Pi(q^2)$  calculated at a definite order. Beyond  $\mathcal{O}(\alpha_s^2)$  complete analytical results for the heavy quark correlator would be cumbersome and only numerical approaches may be available. In this sense, it would be convenient to have a method to calculate  $\text{Im}\Pi_{Q\overline{Q}}^{\text{pert}}$  only based on Feynman graphs. We have already sketched such a method in the discussion following (6): we just need to sum up all the massless cut graphs to get  $\text{Im}\Pi_{3g}$ , and then proceed with the dispersion integration that gives the associated dispersive part [10]. For example, at  $\mathcal{O}(\alpha_s^3)$ , the only massless

absorptive part comes from the three-gluon cut in the diagram of Fig. 2a; let us call  $\mathcal{M}_{3g}^{\mu}$  the amplitude producing three gluons from the heavy quark current at lowest order (i.e. through the quark triangle loop in Fig. 3). The massless contribution to the absorptive part of the correlator is then

$$Im \Pi_{3g}(s) = -\frac{1}{6s} \int dR_{3g} \mathcal{M}_{3g}^{\mu} \cdot \mathcal{M}_{3g\mu}^{*}, \qquad (22)$$

with the three-gluon phase space integral defined by

$$\int dR_{3g} \equiv \frac{1}{3!} \frac{1}{(2\pi)^5} \frac{\pi^2}{4s} \int_0^s ds_1 \int_0^{s-s_1} ds_2, \qquad (23)$$

in terms of the invariants  $s_1 \equiv (k_1 + k_2)^2 = (q - k_3)^2$  and  $s_2 \equiv (k_2 + k_3)^2 = (q - k_1)^2$ , and  $k_i$  being the momenta of the gluons. The real part would be obtained by integrating (22):

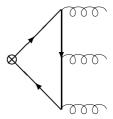
$$\frac{s_0}{\pi} \int_0^\infty \frac{\mathrm{d}s}{s} \frac{\mathrm{Im} \Pi_{3g}(s)}{s+s_0} = \frac{-s_0}{288(2\pi)^4} \int_0^\infty \frac{\mathrm{d}s}{s^3(s+s_0)} \int_0^s \mathrm{d}s_1 \times \int_0^{s-s_1} \mathrm{d}s_2 \mathcal{M}_{3g}^{\mu} \cdot \mathcal{M}_{3g\mu}^*, \tag{24}$$

which, in principle, could be performed also numerically. The *n*th derivative of relation (24) with respect to  $s_0$ , in the limit  $s_0 \to 0^+$ , would give the infrared divergent contribution that should be subtracted from the full moments, as dictated by (21).

Finally, we would like to mention that using the nonrelativistic expansion of the heavy quark correlator in sum rules analyses does not avoid this infrared problem, at least formally. The  $\mathcal{O}(\alpha_s^3)$  diagram of Fig. 2 will be highly suppressed in the velocity expansion, following the nonrelativistic effective field theory approach, and therefore it is not relevant in the corresponding heavy quark currents correlator. However such a two-point function cannot describe the QQ spectrum for energies far from threshold and even when higher n moments, which strongly enhance the threshold, are used, perturbative QCD is needed in order to implement the remaining high energy region; the diagram of Fig. 2 has to be accounted for to properly include this input, and its discontinuity at s=0 cannot be obviated. This point is more clearly seen by noticing that, besides the resummations in  $(\alpha_s/\beta)$  performed in the non-relativistic correlator, one could improve such an expansion by adding the terms needed to reproduce the exact  $\mathcal{O}(\alpha_s^3)$  result  $\Pi(q^2)$ .

#### 6 Conclusions

Heavy quark sum rules, relying on global quark–hadron duality, are a compelling procedure to extract information on the theory from phenomenology. However, as higher perturbative order analyses are performed, the consistency of the method demands the inclusion of novel features. While at  $\mathcal{O}(\alpha_s)$  the correlator of two heavy quark currents gives the full perturbative information, at  $\mathcal{O}(\alpha_s^2)$  we



**Fig. 3.** Feynman diagram for the production of three gluons at  $\mathcal{O}(\alpha_s^3)$ 

have noticed that a heavy quark  $Q\overline{Q}$  pair radiated from light quarks in a correlator of light quark currents should be considered. At  $\mathcal{O}(\alpha_{\rm s}^3)$  the complexities grow with the essential role of non-symmetric correlators. Closely related with this situation is the feature recently pointed out by Groote and Pivovarov of the uneasy problem arising from a massless three-gluon discontinuity in the heavy quark current correlator at  $\mathcal{O}(\alpha_{\rm s}^3)$ .

We have shown that rigorous results of the general theory of singularities of perturbation theory provide all-important tools to analyze the new contributions. The inclusion or exclusion of specific discontinuities on the perturbative side is shown to be feasible and the decision involves a clear definition of the observable input on the phenomenological side of the sum rules.

A solution for the problem pointed out by Groote and Pivovarov at  $\mathcal{O}(\alpha_s^3)$  has been given. We conclude that the appropriate procedure to obtain information about the heavy quark parameters should make use of the infrared safe corrected moments, defined in (21), that now indeed satisfy the modified sum rule

$$\widetilde{\mathcal{M}}_n = \frac{1}{\pi} \int_{4M^2}^{\infty} ds \frac{\operatorname{Im} \Pi_{[Q\overline{Q}]}^{\operatorname{phen}}(s)}{s^{n+1}}, \tag{25}$$

where the right-hand side can be extracted from the heavy quark production cross section  $\sigma(e^+e^- \to [Q\overline{Q}])$ . The uncertainty associated to heavy quark hadronization of the three-gluon should be taken into account but it is shown to be tiny.

The analysis we have carried out is completely general, relying on the theory of singularities of perturbative theory amplitudes only, and provides an adequate tool for the future analysis of heavy quark sum rules.

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