Analytic calculation of doubly heavy hadron spectral density in coordinate space

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Abstract

A systematic and easy-to-use method is developed to calculate directly the doubly heavy hadron spectral density in the coordinate space. The correlation function is expressed in terms of hypergeometric functions, and the spectral density is obtained through two independent approaches: the simple integral representation method and the epsilon-expansion method, respectively. It is found that the spectral density of doubly heavy hadrons can be analytically expressed through commonly known simple functions. This method can drastically simplify and improve the QCD spectral sum rule calculation of the doubly heavy hadrons. An instructive numerical method is also presented for fast evaluation of the spectral density.

Keywords: Sum Rules, Feynman diagrams, Hypergeometric functions

1 Introduction

In the past years, lots of XYZ states [1–3] have been observed by BaBar and Belle collaborations. Many of these states seem not to have a conventional $c\bar{c}$ or $b\bar{b}$ structure, which inspired the extensive study of the exotic hadron spectroscopy. Then many possible structures like tetraquark, hybrid or molecular state are proposed and studied [4–12] with QCD spectral sum rules [13–15].

These structures can be formally expressed as $\{QQ'X\}$, where $Q$ ($Q'$) denotes heavy quark or antiquark and $X$ denotes light quarks and/or gluons. The QCD spectral sum rules require the knowledge of the two-point correlation function or its discontinuity, the spectral density, to study many fundamental properties of hadrons. Spectral density is the most labor-intensive part of the QCD spectral sum rule calculation. Therefore, it is important and helpful to develop a systematic and easy-to-use method to calculate doubly heavy hadron spectral density.

For a hadron state of light quarks and/or gluons, the correlation function can be easily calculated by a Fourier transformation in the coordinate space [16, 17], because the light quark/gluon masses are relatively small and the propagators can be approximated by fractional functions. Once the heavy quarks are introduced into this kind of states, one need either to use the momentum space representation of the heavy quark propagators to keep the masses finite and then evaluate momentum integrals [4, 18], or to handle Bessel function related integrals in coordinate space [19].

In recent years, the momentum space method [4, 18] has been widely used for mesons [4–6, 8, 20–25] and baryons [26] at the leading order in $\alpha_s$. Even so, it is tedious to evaluate two-loop momentum integrals with the traditional methods, especially for integrals with tensor structures. What’s more,

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the double integral representations are time-consuming and might introduce noticeable errors to the sum rules.

In this work, a direct and simple method of analytically calculating the doubly heavy hadron spectral density in the coordinate space is developed. In this method, the heavy quark propagator is expressed in the form of the modified Bessel function of the second kind, and the correlation function can be expressed by a few generalized hypergeometric functions. The hypergeometric representations make the correlation function easily expressed in a compact form and the spectral density easy to be worked out analytically. Note that the negative dimensional integration method (NDIM) [27–29] or its optimized version, the method of brackets (MB) [30–33], is used to calculate some important integrals.

In Refs. [19, 34, 35], the spectral density is calculated in several special cases, where small momentum expansion \( q^2 \to 0 \), large momentum expansion \( q^2 \to -\infty \) and threshold expansion are used to simplify the calculation. Obviously, the spectral density calculated in these special cases is not valid for a wide energy region of the QCD spectral sum rules calculation.

In this work, the spectral density that valid for a wide energy region is calculated in two independent approaches: the simple integral representation method and the \( \epsilon \)-expansion method, respectively. The simple (onefold) integral representation [34] of \( q+1F_q \) type hypergeometric functions is suitable for spectral density calculation, where the knowledge of the power function’s discontinuity is enough to obtain the result. In the recent decade, lots of algorithms or packages [36–42] have been developed to perform the \( \epsilon \)-expansion of hypergeometric functions. Practically, HypExp [38, 39] is used to perform \( \epsilon \)-expansion of \( q+1F_q \) type hypergeometric functions. It is found that the spectral density of doubly heavy hadrons can be analytically expressed in terms of commonly known simple functions and no parameter integral is needed at all.

The well regularized hypergeometric representation of the spectral density can be evaluated numerically, too. An instructive method is developed for numerical computation of the spectral density. In this method, no analytic \( \epsilon \)-expansion is needed, and one can treat hypergeometric functions as common functions. Consequently, the spectral density can be computed directly, which will be helpful to the standard community.

Generally, the coordinate space method can be widely applied to the QCD spectral sum rule calculations of doubly heavy hadron states \( \{QQ'X\} \). This method provides a systematic and easy-to-use approach to calculate directly the doubly heavy hadron spectral density in the coordinate space, which drastically simplifies the QCD spectral sum rule calculation. Expressing the spectral density in terms of simply functions makes the QCD sum rule calculation extremely efficient. There is no noticeable errors from multi-dimensional numerical integrals, either. Then a Monte-Carlo based uncertainty analysis [43, 44] is feasible to make realistic uncertainty estimates of the phenomenological parameters. As the tetraquark or molecular structure of these states leads to (almost) the same predictions within the accuracy [7], such analysis can quantitatively improve the predictive ability of QCD sum rules. Moreover, this method can also serve to be an important cross-check of the widely used momentum representation method.

The paper is organized as follows. After a brief introduction of the traditional momentum space method in the next section, the method of calculating the doubly heavy hadron spectral density in the coordinate space is presented in detail in Sec. 3. The compact hypergeometric representation of the correlation function is derived in Sec. 3.2. Then two approaches to extract discontinuities from the hypergeometric functions are provided in Sec. 3.3 and Sec. 3.4, respectively. In Sec. 4, a concrete calculation is performed to show how to apply the coordinate space method to the practical problems. In Sec. 5, an instructive numerical method is also presented for fast evaluation of the spectral density from the \( \epsilon \)-regularized hypergeometric functions. Finally, a summary is given in Sec. 6.
2 The momentum space method

The QCD spectral sum rules use the two-point correlation functions like

$$\Pi_{\mu\nu}(q) = i \int d^4x e^{iq\cdot x} \langle 0 | T\{j_\mu(x)j_\nu^\dagger(0)\} | 0 \rangle$$

(1)

to study lots of properties of hadrons. Generally, the correlator in coordinate space can be expressed as a product of full propagators and/or their derivatives [19]. And then the correlation function in the momentum space can be expressed as a Fourier transformation of the product of several propagators. For example, the Lorentz invariant two-point correlation function of \{QQqq\} state in coordinate space is of the simple form

$$\Pi(q^2) \sim i \int d^Dx e^{iq\cdot x} S_Q(x)S_Q(-x)S_Q(x)S_Q(-x),$$

(2)

where all color indices, flavor indices and gamma matrices are ignored, for the sake of brevity. The discontinuity of $$\Pi(q^2)$$ is the spectral density, which is needed by the QCD spectral sum rules calculation.

In the past years, the discontinuity of this type of integrals is calculated for mesons \([4–6, 8, 20–25]\) and baryons \([26]\) at the leading order in $$\alpha_s$$ by using the techniques in Ref. \([4, 18]\). To keep the heavy quark mass finite, the momentum space expression of the heavy quark propagator \([15]\)

$$iS^b_Q(p) = \frac{i\delta^{ab}}{\hat{p} - m} + \frac{i\lambda^n_{ab}}{2} g_\mu\nu G^\mu\nu (\hat{p} + m) + (\hat{p} + m) \sigma^{\mu\nu}$$

$$+ \frac{i\delta^{ab}}{12} (g_2^2 G^2) m p^2 + m\hat{p} + \cdots$$

(3)

is used, where $$\hat{p} = \gamma_\mu p^\mu$$. The light quark part of the correlation function is calculated in the coordinate space, and then the whole expression is converted to the momentum space by a D dimensional Fourier transformation. Finally, the two-loop momentum integral is calculated and the spectral density is expressed as double integrals of Feynman or Schwinger parameters.

The two-loop momentum integral is of the form

$$\int \frac{d^4k_1 d^4k_2}{(2\pi)^8} \frac{\mathcal{N}(k_1, k_2, q, m)}{[-k_1^2 + m^2]^{n_1} [-k_2^2 + m^2]^{n_2} [-q - k_1 + k_2]^2]^{n_3}}$$

(4)

It is tedious to calculate this type of integrals in the traditional manner, and the non-trivial numerator $$\mathcal{N}(k_1, k_2, q, m)$$ makes the calculation even complicated. Besides, the double integral representations of Feynman or Schwinger parameters are time-consuming and might introduce noticeable errors to the sum rules. One can also use the Mellin-Barnes method to express such integrals as combinations of hypergeometric functions, but the tensor structure makes the final expression diffuse. Therefore, it is of great significance to find a convenient way of calculating the spectral density.

Actually, the spectral densities of doubly heavy hadrons can be calculated in a straightforward way in the coordinate space. In the following section, a direct and simple method is developed to calculate the doubly heavy spectral density in the coordinate space.

3 The coordinate space method

Since the correlation function can be expressed as the Fourier transformation of a product of propagators in the coordinate space, it is natural to calculate the correlation function in the coordinate space. The light quark propagator and the gluon propagator can be expressed as common functions, because the masses are small and the small mass expansion can be used. As for the heavy quark,
the modified Bessel function of the second kind $K_n(mx)$ is needed to express the propagator in the coordinate space. Note that the so-called fixed-point gauge $(x^\mu A_\mu(x) = 0)$ technique is used to get the full propagators.

### 3.1 Propagators

The free-standing part of the light quark propagator in the coordinate space is [16, 17, 44]

$$iS_q^{ab}(x) = \frac{\delta^{ab}}{2\pi^2 x^4} - \frac{\delta^{ab}}{12} \langle \bar{q}q \rangle - \frac{\delta^{ab} g^2 x^2 \bar{x} \langle \bar{q}q \rangle}{25 \times 3^5} + \frac{\delta^{ab} x^2}{192} \langle g_s \bar{q}q Gq \rangle$$

$$+ \frac{1}{32\pi^2} g \sigma^{\mu\nu} \bar{x} \sigma^{\mu
u} + \frac{\delta^{ab} x^2 \bar{x} \langle \bar{q}q \rangle}{2^7 \times 3^5} + \cdots$$

where $x \equiv i\gamma_\mu x^\mu$ and $G_{\mu\nu}^{ab} \equiv G_{\mu\nu}^a T_{ab}^n = G_{\mu\nu}^n \lambda_{ab}^n/2$. There is also a dangling-gluonic part [17, 44]

$$iS_{q,\mu\nu}^{ab,n}(x) \equiv \langle 0|T \{ g^a(x) g_s \sigma_{\mu\nu} \bar{q}Gq(0) \}|0 \rangle$$

$$= - \frac{1}{2^6 \times 3} \sigma_{\mu\nu} T_{ab}^n \langle g_s \bar{q}q Gq \rangle$$

$$+ \frac{1}{2^5 \times 3} (\sigma_{\mu\nu} \bar{x} + \bar{x} \sigma_{\mu\nu}) T_{ab}^n \langle g_s \bar{q}q Gq \rangle + \cdots,$$

which is important for the condensate contributions from different quarks.

The heavy quark propagator in the coordinate space can be obtained from the Fourier transformation of $iS_Q^{ab}(p)$ in (3),

$$iS_Q^{ab}(x) = \int \frac{d^3p}{(2\pi)^3} iS_Q^{ab}(p) e^{-ipx}.$$

By using the Fourier transformation relation in $D$ dimensional Minkowski space

$$i \int_\mathbb{M} \frac{d^Dp}{(2\pi)^D} \frac{e^{-ipx}}{p^2 - m^2} = \frac{m^{D-2}r^{D-2}/D2K_{D/2}(r)}{(-2)^{-1}(2\pi)^{D/2} \Gamma(D/2)},$$

where $K_\nu(r)$ is the modified Bessel function of the second kind, the heavy quark propagator in the coordinate space can be expressed as

$$iS_Q^{ab}(x) = \frac{m^3 \delta^{ab}}{2\pi^2} \left\{ r^{-2} K_2(r) + r^{-1} K_1(r) \right\}$$

$$- \frac{m_g G_{\mu\nu}^{ab}}{8(2\pi)^2} \left\{ \left( \sigma^{\mu\nu} \bar{r} + \bar{r} \sigma^{\mu\nu} \right) r^{-1} K_1(r) + 2 \sigma^{\mu\nu} K_0(r) \right\}$$

$$- \frac{\delta^{ab} (g^2 G^2)}{576(2\pi)^2} \left\{ (\bar{r} - 6) r^1 K_1(r) + r^2 K_2(r) \right\} + \cdots,$$

where $\bar{r} \equiv m \bar{x}$, $r \equiv m \sqrt{-x^2}$ and $r^2 = r^2$. 

4
In the coordinate space, components of the light quark propagator (5) are of the form \((-x^2)^n\) or \(\bar{x}(-x^2)^n\). Note that the \((-x^2)^{n-2} \ln(-x^2)\) terms can be rewritten in the form of \((-x^2)^{n-D/2} \Gamma(D/2 - n)\). As for the heavy quark propagator (9), components are of the form \((-x^2)^n K_\nu(m\sqrt{-x^2})\) or \(\bar{x}(-x^2)^n K_\nu(m\sqrt{-x^2})\). Naturally, the correlation function (2) can be expressed as \(D\) dimensional Fourier transformation of two Bessel functions.

3.2 Hypergeometric representation of the correlation function

After some algebras of the Dirac gamma matrices, the Gell-Mann matrices and the color indices [45], the correlation function reads

\[
\Pi^{\mu\nu}(q) \sim i \int_M d^D x e^{iq.x} \{-g^{\mu\nu}, x^\mu x^\nu\} \sum_i \sqrt{-x^2} K_{\nu_1} (m\sqrt{-x^2}) K_{\nu_2} (m\sqrt{-x^2}),
\]  

(10)

where \(-g^{\mu\nu}, x^\mu x^\nu\) are possible Lorentz structures and “M” indicates the above integral is calculated in the Minkowski space. The angular integral of the Fourier transformation is trivial,

\[
i \int_M d^D x e^{iq.x} f(\sqrt{-x^2}) = (2\pi)^{D/2} Q^{1-D/2} \int_0^\infty dx x^{D/2} J_{D/2-1}(Qx) f(x),
\]  

(11)

where \(Q^2 = -q^2\), \(Q > 0\), and \(J_\nu(x)\) is the Bessel function of the first kind.

Consequently, the correlation function \(\Pi(q^2)\) turns into one dimensional integrals of one Bessel \(J\) and two Bessel \(K\)’s:

\[
\int_0^\infty dx x^{u-1} J_\nu(Qx) K_\alpha(mx) K_\beta(mx).
\]

This type of integrals can be worked out analytically with the help of negative dimensional integration method (NDIM) [27–29] or its optimized version, the method of brackets (MB) [30–33]. In this calculation, Bessel functions are needed to be expressed in the form of series. In detail,

\[
J_\nu(x) = \frac{\phi_m}{\Gamma(m + \nu + 1)} \left(\frac{x}{2}\right)^{2m+\nu},
\]  

(12)

where \(\phi_m = \frac{(-1)^m}{\Gamma(m+1)}\). Since \(K_\nu(x)\) does not have a single summation series representation, one needs to express \(K_\nu(x)\) as a definite integral

\[
K_\nu(x) = \frac{1}{2} \int_0^\infty dt t^{\nu-1} e^{-\frac{t}{2}(t+1)},
\]  

(13)

or as a double summation series

\[
K_\nu(x) = \frac{1}{2} \sum_{n_1, n_2} \phi_{n_1, n_2} \left(\frac{x}{2}\right)^{n_1+n_2} (n_1 - n_2 + \nu),
\]  

(14)

where \(\phi_{n_1, n_2} = \phi_{n_1}\phi_{n_2}\) and a formal symbol \(\langle a \rangle\), the bracket, is introduced. This bracket is a short form of the divergent integral

\[
\int_0^\infty dx x^{a-1} = \langle a \rangle.
\]  

(15)

After a little algebra, one gets the key integral of the correlation function calculation in coordinate
the hypergeometric functions.

\[
\int_0^\infty dx \, x^{u-1} J_v(Qx)K_a(mx)K_b(mx)
= 2^{u-3}m^{-u-v}Qv \frac{\Gamma(A_-)\Gamma(A_+)\Gamma(A_{++})}{\Gamma(1+v)\Gamma(u+v)}
\times {}_4F_3\left( \begin{array}{cccc}
A_-, A_+, A_{++}, A_{++} \\
1+v, u+v, \frac{1+u+v}{2}, \frac{1+u+v}{2} \end{array} \bigg| -\frac{Q^2}{4m^2} \right).
\]

(16)

Here the notation

\[
A_{\lambda_1\lambda_2} \equiv \frac{u + v + \lambda_1 a + \lambda_2 b}{2}
\]

is used to keep the expression short. A similar integral with one Bessel \( K \) has been given in the form of \( {}_3F_1 \) in Ref. \[19\], which can be used to study hadrons with one heavy quark like \( D \) and \( B \) mesons as well as \( \Lambda_c \) and \( \Lambda_b \) baryons. Since Feynman integrals can be expressed as linear combinations of hypergeometric functions, and two-loop self-energy integrals as well as two-loop sunset-type diagrams have \( {}_4F_3 \) representations \[34, 46\], the above expression appears as expected.

Alternatively, the integral above can also be expressed as

\[
\int_0^\infty dx \, x^{u-1} J_v(Qx)K_a(mx)K_b(mx)
= 2^{u-3}m^{a+b}Q^{-u-a-b} \frac{\Gamma(-a)\Gamma(-b)\Gamma(\frac{u+v+a+b}{2})}{\Gamma(1 - \frac{u+a+b}{2})}
\times {}_4F_3\left( \begin{array}{cccc}
\frac{1+a+b}{2}, \frac{1}{2}, \frac{u+a+b}{2}, \frac{u+v+a+b}{2} \\
1 + a, 1 + b, 1 + a + b \end{array} \bigg| \frac{4m^2}{-Q^2} \right)
+ (a \rightarrow -a) + (b \rightarrow -b) + (a \rightarrow -a, b \rightarrow -b).
\]

(17)

These two representations (16) and (17) are simply related to each other by analytic continuation of the hypergeometric functions.

\[
q+1F_q\left( \begin{array}{c}
a_1, \ldots, a_{q+1} \\
b_1, \ldots, b_q \end{array} \bigg| z \right)
= \frac{\Gamma(b_1) \cdots \Gamma(b_q)}{\Gamma(a_1) \cdots \Gamma(a_{q+1})} \sum_{j=1}^{q+1} \frac{\Gamma(a_j) \prod_{j=1}^{q+1} \Gamma(a_j - a_i)}{\prod_{j=1}^{q+1} \Gamma(b_j - a_i)}
\times (-z)^{-a_i q+1F_q\left( \begin{array}{c}
a_i, \{1 + a_i - b_k\}_{k=1,\ldots,q} \\
\{1 + a_i - ak\}_{k=1,\ldots,q+1;k \neq i} \end{array} \bigg| \frac{1}{2} \right),
\]

(18)

where \( a_i - a_i \notin \mathbb{Z} \). In the following calculation, (16) is used to derive the hypergeometric representation of the correlation function because this representation can be simply regularized by performing the coordinate space integral in \( D = 4 - 2\epsilon \) dimension.

Using (11) and (16), the hypergeometric representation of the correlation function can be worked out as

\[
PK_0 = i \int_M d^Dx \, e^{iqx} \sqrt{-x^2} K_a(m\sqrt{-x^2})K_b(m\sqrt{-x^2})
= 2^{D+w-2} \pi^{D/2} \Gamma(B_{--})\Gamma(B_{+-})\Gamma(B_{-+})\Gamma(B_{++})
\times m^{D+w} \frac{\Gamma(\frac{D}{2})\Gamma(D+w)}{\Gamma(D+w)}
\times {}_4F_3\left( \begin{array}{cccc}
B_{--}, B_{+-}, B_{-+}, B_{++} \\
\frac{D}{2}, \frac{D+w}{2}, \frac{D+w+1}{2} \end{array} \bigg| z \right).
\]

(19)
where \( z = s/(4m^2) \) and \( s = q^2 = -Q^2 \). Here the notation

\[
B_{\lambda_1\lambda_2} \equiv \frac{D + w + \lambda_1 a + \lambda_2 b}{2}
\]

is used to keep the expression short. Note that \( D \) appears in every Gamma function and every parameter of the hypergeometric function, which regularizes the divergences very well. It is helpful to use the dimensionless variable \( z \) as the argument of hypergeometric function. Consequently, all dimensional constants like masses and condensates appear in the overall factor. What’s more, \( z \) appears only in the hypergeometric function, which makes it transparent that the correlation function has a discontinuity only for \( z \geq 1 \) (or \( s \geq 4m^2 \)).

In the spectral density calculation, the coordinate space integral is performed in \( D = 4 - 2\epsilon \) dimension, while the propagators of light and heavy quarks in 4 dimension are employed. That is, \( w \), \( a \) and \( b \) in (19) are all integers. The dimension parameter \( D \) in the power of constants like \( 2^{D+w-2} \), \( \pi^{D/2} \) and \( m^{D+w} \) can be set to 4 safely, because the \( \epsilon \) related higher-order infinitesimal terms of the constant coefficients will not lead to finite contributions to the spectral density. Furthermore, \( _4F_3 \) will reduce to \( _3F_2 \) or even much simpler functions, depending on the specific situation.

The correlation function contains Lorentz indices \( \mu \) and \( \nu \), which means \( \Pi_{\mu\nu} (x) \) contains \( g_{\mu\nu} \) and \( x_\mu x_\nu \) structures, as mentioned in (10). Terms proportional to \( g_{\mu\nu} \) can be directly calculated through (19), and terms proportional to \( x_\mu x_\nu \) can be calculated through the differential form of (19).

The derivative of hypergeometric function is

\[
\frac{\partial}{\partial z} q_1 F_q \left( \{a_i\}, \{b_j\} \bigg| z \right) = \frac{\Pi\{a_i\}}{\Pi\{b_j\}} q_1 F_q \left( \{a_i + 1\}, \{b_j + 1\} \bigg| z \right),
\]

where \( \Pi\{a_i\} = \Pi_{i=1}^{q+1} a_i \) and \( \Pi\{b_j\} = \Pi_{j=1}^{q} b_j \). The double partial derivative of hypergeometric function is

\[
- \frac{\partial^2}{\partial q_\mu \partial q_\nu} _4 F_3 \left( \{a_i\}, \{b_j\} \bigg| \frac{q^2}{4m^2} \right) = - \frac{g^{\mu\nu}}{2m^2} _4 F_3 \left( \{a_i + 1\}, \{b_j + 1\} \bigg| \frac{q^2}{4m^2} \right).
\]

For the hadron state with \( J^{PC} = 1^{++} \), only the \((-g^{\mu\nu})\) part is needed in the spectral density calculation. As a result, one gets

\[
PK_2 = i \int_M d^D x e^{i a_i x^\mu} x^\nu \sqrt{-x^2}^{w-2} K_0(m\sqrt{-x^2}) K_i(m\sqrt{-x^2})
\]

\[
\times 2^{D+w-3} \pi^{D/2} \Gamma(B_{--}) \Gamma(B_{+-}) \Gamma(B_{++}) m^{D+w} \Gamma(1 + \frac{D}{2}) \Gamma(D + w)
\]

\[
\times _4 F_3 \left( B_{--}, B_{+-}, B_{-+}, B_{++} \bigg| 1 + \frac{D}{2}, \frac{D+w}{2}, \frac{D+w+1}{2} \bigg| z \right).
\]

Note that the factor \((-g^{\mu\nu})\) is omitted here for the sake of simplicity.

By using (19) and (20), one can carry out the hypergeometric representations of the correlation function \( \Pi_1 (q^2) \). The parameters \( \{a_i\} \) and \( \{b_j\} \) of \( q_1 F_q (\{a_i\}, \{b_j\}, z) \) type hypergeometric functions are linear functions of space-time dimension \( D = 4 - 2\epsilon \), where \( \epsilon \) regulates UV and/or IR divergences.

In fact, it is not too hard to express some integrals as generalized hypergeometric functions, because it is trivial, to some extent, to transform these integrals into summands. Nevertheless, if these hypergeometric functions cannot be easily handled, they are nothing more than short notations and the problem remains unsolved. Fortunately, with the help of some new technologies, the \( q_1 F_q \) type hypergeometric functions can be effectively handled in many ways.
To extract the spectral density form the hypergeometric representation of the correlation function, two independent approaches are presented below. The simple integral representation method in Sec. 3.3 is easy-to-use, where the spectral density will be expressed as one-dimensional integrals. In Sec. 3.4, the $\epsilon$-expansion method of the hypergeometric functions can even express the spectral density in terms of some commonly known functions and no integral is needed.

### 3.3 Integral representation of hypergeometric function

Once the correlation function is expressed as hypergeometric functions like in (19) and (20), one can use the simple integral representations [34] of $2F_1$ and $3F_2$

\[
2F_1 \left( \begin{array}{l} a_1, a_2 \\ b_1 
\end{array} \right) = \frac{\Gamma(b_1)}{\Gamma(a_2)\Gamma(b_1-a_2)} \int_1^{\infty} dt \frac{t^{a_1-b_1}(t-1)^{b_1-a_2-1}}{(t-z)^{a_1}},
\]

\[
3F_2 \left( \begin{array}{l} a_1, a_2, a_3 \\ b_1, b_2 
\end{array} \right) = \frac{\Gamma(b_1)\Gamma(b_2)}{\Gamma(a_2)\Gamma(a_3)\Gamma(b_1+b_2-a_2-a_3)} \int_1^{\infty} dt \frac{t^{a_1-b_1}(t-1)^{b_1+b_2-a_2-a_3-1}}{(t-z)^{a_1}} \times 2F_1 \left( \begin{array}{l} b_2-a_2, b_2-a_3 \\ b_1+b_2-a_2-a_3 
\end{array} \right) \frac{1-t}{1-t},
\]

to calculate the spectral density. It is worth noting that these integral representations are peculiarly suitable for the discontinuity calculation. In these representations, $z$ only appears in $(t-z)^{-a_1}$. Generally, the discontinuity of $(t-z)^{-a_1}$ is [19]

\[
\frac{1}{2\pi i} \text{Disc}(t-z)^{-a_1} = \frac{(z-t)^{-a_1}\theta(z-t)}{\Gamma(a_1)\Gamma(1-a_1)}.
\]

Note that for $a_1 = n - \epsilon$, where $n$ is a positive integer, the expansion [47, 48]

\[
z^{\epsilon-1} = \frac{1}{\epsilon} \delta(z) + \sum_{m=0}^{\infty} \frac{\epsilon^m}{m!} \left[ \log^m \left( \frac{z}{z} \right) \right] +
\]

and its differential forms are used to calculate the discontinuities of the above integrals. The “plus” distributions are defined as

\[
\int dz \ f(z) \left[ \log \left( \frac{z}{z} \right) \right]_+ = \int dz \ (f(z) - f(0)) \frac{g(z)}{z}.
\]

For the high dimensional condensate parts of the correlation function, $B_{\lambda_1\lambda_2}$ may be positive. The “delta” distribution is more important than the “plus” one, because it will lead to $\epsilon^{-1}\delta^{(n)}(z-t)$ type of contributions to the simple integral. Note that the surface terms of the $\delta^{(n)}(z-t)$ related integrals may contain finite contributions to the sum rules.

If the hypergeometric functions have already reduced to some simple functions like $(z-1)^{-n}$, where $n$ is a positive integer, no integral representation is needed and the discontinuity can be calculated as follows

\[
\frac{1}{2\pi i} \text{Disc}(-z)^{-n} = \frac{1}{(n-1)!} \delta^{(n-1)}(z).
\]

### 3.4 Epsilon expansion of hypergeometric function

The spectral density can even be analytically worked out from the hypergeometric representation of the correlation function. In the recent decade, lots of algorithms and packages [36–42] have been
developed to perform the ε-expansion of hypergeometric functions. Among them, HypExp [38, 39] provides a systematic and easy-to-use approach to perform ε-expansion of $F_{g+1}$ type hypergeometric functions, whose parameters $\{a_i\}$ and $\{b_j\}$ are of the form $n + \alpha \epsilon$ or $n + n_{i-} + \alpha \epsilon$.

In (19) and (20), the overall factor of Gamma functions has non-zero contribution from order $O(\epsilon^{-n_1})$, while hypergeometric function has non-zero discontinuity from order $O(\epsilon^{n_2})$. For the calculations in Sec. 4, it is interesting to see that $n_1 = n_2$, and then the spectral density calculation can be drastically simplified by only calculating $\epsilon^{-n_1}$ part of the overall factor and $\epsilon^{n_1}$ part of the hypergeometric function. Perhaps this favorable condition does not always exist, but it is worth checking it beforehand.

After ε-expansion, the hypergeometric functions (or the correlation functions) are expressed in terms of commonly known functions and harmonic polylogarithms (HPLs) [49, 50]. The HPLs are of the form

$$H_{\ldots} \left( i\sqrt{\frac{z}{z-1}} \right),$$

where $\ldots$ denotes indices. Note that the argument $i\sqrt{-z/(z-1)}$ of HPLs is not in the well-defined interval $(0, 1)$ for $z > 1$, one cannot naively convert this kind of HPLs to commonly known functions for now.

Empirically, it is preferable to keep the HPLs unchanged before the discontinuities are worked out because HPLs are compact functions. Otherwise, one need to calculate the discontinuities of a large amount of common functions. The discontinuities are calculated through

$$\rho(z) = \frac{1}{2\pi i} \text{Disc} \Pi(z) = \lim_{\epsilon \to 0^+} \frac{\Pi(z + i\epsilon) - \Pi(z - i\epsilon)}{2\pi i}.$$

Particularly,

$$\sqrt{\frac{z}{z-1}} \equiv \epsilon \pm i \sqrt{\frac{z}{z-1}}, \quad \text{for } z > 1,$$

and now the argument of HPLs becomes $-\sqrt{z/(z-1)} + i\epsilon$ or $\sqrt{z/(z-1)} + i\epsilon$, respectively.

Since the HPLs are well defined for arguments in the interval $(0, 1)$ [39, 50, 51], while the real parts $-\sqrt{z/(z-1)} \in (-\infty, -1)$ and $\sqrt{z/(z-1)} \in (1, \infty)$, these HPLs need to be analytically continued to the interval $(0, 1)$ before converting them into commonly known functions. The analytic continuation sign $\delta$ in the small imaginary part $i\delta \epsilon$ of the argument is important. In the practical calculation, HPLs with argument $-\sqrt{z/(z-1)} + i\epsilon$ are analytically continued from $(-\infty, -1)$ to $(0, 1)$ by the function

$$\text{HPLAnalyticContinuation}[#, \text{AnalyticContinuationSign} -> 1, \text{AnalyticContinuationRegion} -> \text{minftom1}] &$$

and HPLs with argument $\sqrt{z/(z-1)} + i\epsilon$ are analytically continued from $(1, \infty)$ to $(0, 1)$ by the function

$$\text{HPLAnalyticContinuation}[#, \text{AnalyticContinuationSign} -> 1, \text{AnalyticContinuationRegion} -> \text{onetoinf}] &$$

After the analytic continuation, the argument of all HPLs becomes $\sqrt{1-1/z}$, which is in the interval $(0, 1)$ for $z > 1$. Now one can use (28) to calculate the discontinuity of the ε-expanded expression. It is known from the practical calculations that only a few HPLs (see (43)) are needed to express the spectral density in a neat form. Since the argument of all HPLs becomes $\sqrt{1-1/z} \in (0, 1)$ for $z > 1$, it is safe to convert HPLs to commonly known functions like logarithm or polylogarithm. Besides, HPLs can also be numerically evaluated with high efficiency like the common functions [50], and one can directly use HPLs in the numerical calculation.
The discontinuity near the lower threshold \( z = 1 \) is related to functions of the form \((1 - z)^{-a}\). If \( a \) is a positive integer, one can use (26) to calculate the discontinuity. The balance parameter

\[
\sigma = \sum_{j=1}^{q} b_j - \sum_{i=1}^{q+1} a_i
\]

(30)
is used to determine the \( z \to 1 \) behavior of \( q_{r+1} F_q \) type hypergeometric functions \[52, 53\]. If \( \sigma < 0 \), the singular parts of the hypergeometric function are of the form \((1 - z)^{\sigma + k}\), an additional regularization is needed to cancel such kind of divergences. Such contributions might appear when the higher dimensional condensates are taken into consideration. From (19) and (20), it is easy to see that \( \sigma = (1 - D)/2 - w \) or \( \sigma = (3 - D)/2 - w \). Since \( w \) is an integer and \( D \) will be set to 4 after the \( \epsilon \)-expansion, \( \sigma \) cannot be a negative integer. As a result, \((1 - z)^{-n}\) will not appear in the correlation function, and the spectral density will not contain Dirac delta function related terms, either.

4 Application

In this section, a concrete calculation is performed to show that the spectral density of doubly heavy hadrons like hidden-charm tetraquark state \[4\] can be easily obtained by using the coordinate space method.

The two-point correlation function (1) in the QCD spectral sum rules can be decomposed into two parts as

\[
\Pi_{\mu \nu}(q) = \left( \frac{q_{\mu}q_{\nu}}{q^2} - g_{\mu \nu} \right) \Pi_1(q^2) + \frac{q_{\mu}q_{\nu}}{q^2} \Pi_0(q^2).
\]

(31)

\( \Pi_1(q^2) \) and \( \Pi_0(q^2) \) have the quantum numbers of the spin 1 and 0 mesons, respectively. For the QCD spectral sum rule calculation of \( X(3872) \) meson state with \( J^{PC} = 1^{++} \), only \( \Pi_1(q^2) \) is of interest. The correlation function and the spectral density are related by a dispersion relation

\[
\Pi_1(q^2) = \int_{s_<}^{\infty} ds \frac{\rho(s)}{s - q^2},
\]

(32)

where \( s_< \) is the lower threshold and the spectral density is the discontinuity of the correlation function

\[
\rho(s) = \frac{1}{2\pi i} \text{Disc} \Pi_1(s).
\]

(33)

The current of the \( 1^{++} \) tetraquark \([qc][\bar{q}c]\) is given by \[4\]

\[
{j}_\nu = f_{abcde} (q_a^T C\Gamma^A c_b)(\bar{q}_d \Gamma^B C\bar{c}^T_e),
\]

(34)

where \( f_{abcde} \) is the color structure factor, and the Dirac gamma matrix \( \Gamma \) is of the form \( I, \gamma^\mu, \sigma^{\mu \nu}, \gamma^5 \gamma^\mu \) or \( i\gamma^5 \). Note that \( \Gamma \)’s satisfy the transformation relation

\[
\gamma^0 \Gamma^\dagger \gamma^0 = \Gamma^T.
\]

(35)

The vacuum expectation value of the currents is

\[
\langle 0 | T \{ j_\mu(x) j^\dagger_\nu(0) \} | 0 \rangle = \langle 0 | T \{ j_\mu(x) j^\dagger_\nu(0) \} | 0 \rangle_1 + (\Gamma^A \leftrightarrow \Gamma^B) + (\Gamma^C \leftrightarrow \Gamma^D) + (\Gamma^A \leftrightarrow \Gamma^B, \Gamma^C \leftrightarrow \Gamma^D).
\]

(36)
The labeled gamma matrices $\Gamma^A$, $\Gamma^B$, $\Gamma^C$ and $\Gamma^D$ are introduced to make the sources of the gamma matrices explicit. In the final expression, these gamma matrices will be replaced by $i\gamma_5$, $\gamma_\mu$, $i\gamma_5$ and $\gamma_\nu$, respectively, for the specific spectral density calculation in Ref. [4].

After contracting the quark fields in the correlation function with Wick theorem, one part of the vacuum expectation values reads

$$
\langle 0| T \{ j_\mu (x) j_\nu^\dagger (0) \} | 0 \rangle_1 = \langle 0 | \text{Tr} \{ \Gamma^A [iS_{bb}^q (x)] \Gamma^C (C[iS_{aa}^q (x)]^T C^{-1}) \} \times \text{Tr} \{ \Gamma^B (C[iS_{ee}^q (-x)]^T C^{-1}) \Gamma^D [iS_{dd}^q (-x)] \} | 0 \rangle,
$$

where $iS_{aa}^q (x)$ is the full quark propagator in coordinate space. It is easy to obtain the other three parts by permutations of gamma matrices.

In the propagators (5) and (9), the gamma matrix related structures are $1$, $\bar{x}$, $\sigma^{\mu\nu}$, $\sigma^{\mu\nu} \vec{x} + \vec{x} \sigma^{\mu\nu}$. Their charge conjugation transformations are

$$
C \{ 1, \bar{x}, \sigma^{\mu\nu}, \sigma^{\mu\nu} \bar{x} + \bar{x} \sigma^{\mu\nu} \} C^{-1} = \{ 1, -\bar{x}, -\sigma^{\mu\nu}, \sigma^{\mu\nu} \bar{x} + \bar{x} \sigma^{\mu\nu} \}.
$$

With the help of this identity, it is easy to get the charge conjugation of the quark propagators. After some algebras of the gamma matrices, the Gell-Mann matrices and the color indices [45], the correlation function can be obtained easily. For example, the perturbative part of the correlator in coordinate space is

$$
\Pi^\text{pert.}^{\mu\nu}_1 (x) = \frac{3m^4}{\pi^5} (-g^{\mu\nu}(-x^2)^{-4} - 2x^{\mu}x^{\nu}(-x^2)^{-5}) K_{-2}(m_c \sqrt{-x^2})^2.
$$

By using (19) and (20) with $w = -8$ and $a = b = -2$, one gets the $\Pi^\text{pert.}_1 (z)$ in the form of hypergeometric functions. Explicitly,

$$
\Pi^\text{pert.}_1 (z) = \frac{3m^5}{64\pi^8} \left\{ \frac{\Gamma(-\epsilon - 4)\Gamma(-\epsilon - 2)\Gamma(-\epsilon)}{\Gamma(2 - \epsilon)\Gamma(-2\epsilon - 4)} \right. 3F_2 \left( \begin{array}{c} -\epsilon - 4, -\epsilon - 2, -\epsilon \\ -\epsilon - \frac{3}{2}, 2 - \epsilon \end{array} \right) \left. \frac{z}{13} \right\}.
$$

With the help of (22) and (23), one gets the simple integral representation of the perturbative part of the spectral density

$$
\rho^\text{pert.} (z) = \frac{m^8}{\pi^9} \left\{ \frac{32}{345} \int_1^{\infty} dt \frac{t^{3/2}(t - 1)^{11/2}}{112} 2F_1 \left( \begin{array}{c} \frac{5}{12} \\ \frac{13}{4} \end{array} \right) 1 - t \right\} - \frac{64}{45045} \int_1^{\infty} dt \frac{t^{3/2}(t - 1)^{13/2}}{112} 2F_1 \left( \begin{array}{c} \frac{5}{12} \\ \frac{15}{4} \end{array} \right) 1 - t \right\}.
$$

Here $a_1 = -\epsilon$ is chosen, which makes the $(z - t)^{-a_1}$ trivial when $\epsilon$ expansion is performed. It is worth noting that one has the freedom to chose a parameter from $\{ a_i \}$ as $a_1$, for $\{ a_i \}$ in $\rho^i_{Fq}$ are totally symmetric. With other choices of $a_1$, different but equivalent integral representations will be obtained. Analogously, the other parts of the spectral density can be expressed as simple integrals, too.

Furthermore, the spectral density can also be worked out analytically from (40) by using the $\epsilon$-expansion method in Sec. 3.4. Note that the $\epsilon$-expansion of the Gamma functions in (40) begins from $g_{-3} \epsilon^{-3}$, while the non-vanishing discontinuity of the hypergeometric function $3F_2$ begins from $f_3(z) \epsilon^3$. Technically, it is sufficient to take $g_{-3} f_3(z)$ as the perturbative part of the correlation function, which makes the spectral density calculation drastically simplified. Explicitly, the perturbative part of the
spectral density is
\[
\rho_{\text{pert}}(z) = \frac{m_c^8}{2^{10} \pi^6} \left\{ \frac{32z^4}{9} - \frac{1456z^3}{45} + \frac{776z^2}{15} + \frac{2624z}{45} + \frac{7}{18} + \frac{7}{12z} \right\} V(z) + \left\{ 48z^2 - \frac{128z}{3} + 5 + \frac{7}{24z^2} \right\} U(z) + 12T(z), \tag{42}
\]
where
\[
V(z) = \sqrt{1 - 1/z}, \quad U(z) = H_+(V(z)), \quad T(z) = H_{-,+}(V(z)). \tag{43}
\]
The HPLs [49, 50] \(H_+(z)\) and \(H_{-,+}(z)\) can be converted to commonly known functions
\[
H_+(V(z)) = \log(1 + V(z)) - \log(1 - V(z)), \tag{44}
\]
\[
H_{-,+}(V(z)) = \text{Li}_2 \left( \frac{1-V(z)}{2} \right) - \text{Li}_2 \left( \frac{1+V(z)}{2} \right) + \frac{1}{2} \log(4z)U(z), \tag{45}
\]
where \(\text{Li}_2(z)\) is the Euler dilogarithm.

In Ref. [4], spectral density is calculated by the momentum integral method. The perturbative part of the spectral density is expressed by double integral of modified Feynman or Schwinger parameters
\[
\rho^\text{pert}(s) = \frac{1}{2^{10} \pi^6} \int_{\alpha_<}^{\alpha_>} \int_{\beta_<}^{\beta_>} d\alpha \, \beta \alpha^3 (1 - \alpha - \beta) \left( 1 + \alpha + \beta \right) \left( \alpha - \beta \right) m_c^2 - \alpha \beta s^4, \tag{46}
\]
where \(\alpha_<= (1-v)/2, \alpha_>= (1+v)/2, \beta_<= \alpha m_c^2 / (\alpha - m_c^2)\) and \(\beta_>= 1 - \alpha, \) with \(v = \sqrt{1 - 4m_c^2/s}.\) This double integral representation is obtained by calculating the discontinuity of two-loop sunset type momentum integrals like (4).

\(V(z)\) and \(U(z)\) vary drastically near the threshold \(z = 1,\) which means the numerical computation of the double integral representation (46) might contain large relative errors near the threshold. In the QCD sum rules approach, high energy part of the spectral density \(\rho(z = s/(4m_c^2))\) is damped by the factor \(e^{-zT},\) and the large relative errors of the low energy part of the spectral density might cause some noticeable errors to the sum rules. The double integrals are also time-consuming. Actually, three-fold numerical integrals are involved in the sum rule calculation, if the \(s\) integrals is taken into account. Numerically, (46) is about hundreds of times slower than (42).

To make realistic uncertainty estimates of the results, a Monte-Carlo based uncertainty analysis [43, 44] is often used in the QCD sum rule calculation. In this procedure, the entire phase space of QCD input parameters like quark masses and condensates, is explored simultaneously, and is mapped into uncertainties in the phenomenological parameters. Since a Monte-Carlo based uncertainty analysis need more than 100 times of evaluation to get stable uncertainties, it is not wise to repeatedly calculate the multi-dimensional integrals. Technically, one can write the double integrals in a dimensionless form by taking the dimensional parameters as the coefficients of these integrals. Subsequently, the double integrals can be numerically evaluated only once for a sequence of uniformly-spaced points \(z_i = s_i/(4m_c^2),\) and then the Newton-Cotes formula is used to perform the \(z\) integration.

Comparing (41) and (42) with (46), one can find that the coordinate space method is more suitable for spectral density and sum rule calculation, at least for the case of two heavy quarks with equal masses.

In the same way, the explicit analytic expressions of the other parts of the spectral density [4] can be obtained as
\[
\rho_{m_q}(z) = \frac{m_q m_c^7}{2^{8} \pi^6} \left\{ \frac{48z^3}{5} + \frac{617z^2}{15} - \frac{2087z}{30} - \frac{127}{24z} - \frac{7}{16z^2} \right\} V(z) - \left\{ 28z^2 - 40z - 3 + \frac{5}{2z} + \frac{7}{32z^2} \right\} U(z) - 18T(z) \right\}, \tag{47}
\]
If the parameters \(a\) and \(z\) have no branch cuts, the discontinuities come only from the \((-z)^n\) part. With the help of (23), one gets the discontinuities.

\[
\rho^{(q\bar{q})}(z) = \frac{m^2(q\bar{q})}{2\pi^4} \bigg\{ - \frac{14z^2 + 47z - 41}{9} - \frac{5}{24z} \bigg\} V(z) \\
+ \frac{20z}{3} - \frac{1}{2} + \frac{5}{48z^2} U(z) \bigg\},
\]

(48)

\[
\rho^{(G^2)}(z) = \frac{m^4(g^2G^2)}{2^{b}3^n} \bigg\{ - \frac{4z^2 + 5z - 1}{3} \bigg\} V(z) + \bigg\{ 2z - 1 + \frac{1}{4z} \bigg\} U(z) \bigg\},
\]

(49)

\[
\rho^{\text{mix}}(z) = \frac{m^3(q\bar{q}G_q)}{2^{6}\pi^4} \bigg\{ \frac{58z^2}{9} - \frac{7}{36} - \frac{7}{24z} \bigg\} V(z) - \bigg\{ \frac{4z}{3} + \frac{3}{2} + \frac{7}{48z^2} \bigg\} U(z) \bigg\},
\]

(50)

\[
\rho^{(q\bar{q})^2}(z) = \frac{m^2(q\bar{q})^2}{12\pi^4} V(z).
\]

(51)

Accordingly, the spectral densities of the doubly heavy meson state are analytically worked out through the coordinate space method. Since no multi-dimensional integral like (46) is involved in the spectral density and the analytic functions can be numerically calculated with high efficiency, the errors of sum rules from spectral density functions are minimized. Moreover, a Monte-Carlo based uncertainty analysis can be performed to make realistic uncertainty estimates of the phenomenological parameters, which will improve the predictive ability of QCD sum rules.

5 Numerical evaluation of spectral density

As the hypergeometric functions might not be well known for the standard community and the analytic reduction might be a little involved, a numerical method is presented in this section for fast evaluation of the spectral density from the \(\epsilon\)-regularized hypergeometric functions. Consequently, no analytic \(\epsilon\)-expansion is needed, and the regularization scheme is no longer restricted by the capabilities of HypExp [39].

Since the spectral density itself is finite [54] and independent of the regularization parameter, an unorthodox but reasonable regularization scheme can be used to obtain the spectral density. Formally, the well regularized spectral density can be expressed in the form of

\[
\rho(z, \epsilon) = \sum_{n=1}^{m} \epsilon^{-n} \cdot 0 + \rho(z) + O(\epsilon),
\]

(52)

where \(\rho(z, \epsilon)\) is the approximation of order \(O(\epsilon)\) of the true spectral density \(\rho(z)\). If \(\epsilon\) is numerically small enough, \(\rho(z, \epsilon)\) can be taken as \(\rho(z)\). It is worth noting that multiple precision computation is needed to get rid of roundoff errors from the \(\sum_{n=1}^{m} \epsilon^{-n} \cdot 0\) part. Roughly, \(-(m + 1) \log(\epsilon)\) digits of precision is enough to obtain the correct results.

Practically, (19) and (20) with the regularization parameter \(D = 4 - 2\epsilon\) are not good for numerical computation, because \(q_{+1}F_q(\{a_i\}, \{b_j\}, z)\) is evaluated through its analytic continuation (18) for \(z > 1\). If the parameters \(a_j - a_i \in \mathbb{Z}\), the arguments of gamma functions as well as the parameters of \(q_{+1}F_q(\{a'_i\}, \{b'_j\}, 1/z)\) may contain nonpositive integers, and some spurious divergences may arise. Then, additional auxiliary parameters are needed to regularize the expression, which may lead to a complex calculation.

Using (18), (19) and (20), it is straightforward to get the hypergeometric representation of the correlation function with argument \(1/z\). In this section, this representation will be used for numerical computation. For \(z > 1\), the hypergeometric functions with argument \(1/z\) have no branch cuts, and the discontinuities come only from the \((-z)^n\) part.
of the integrals of \((-g^{\mu\nu})\) and \(x^\mu x^\nu\) structures. Explicitly,

\[
\begin{align*}
\text{DK}_0 &= \frac{1}{2\pi i} \text{Disc} i \int_M d^D x e^{i q \cdot x} \sqrt{-x^2} \ K_a(m\sqrt{-x^2}) K_b(m\sqrt{-x^2}) \\
&= -2^{a-b-2} \pi^{D/2} m^{-D-w-z} \frac{\Gamma(-a)\Gamma(-b)}{\Gamma(1-D-w+a+b+1)\Gamma(-w+a+b)} \\
& \quad \times 4F3 \left( \frac{1+a+b}{2}, 1 + \frac{a+b}{2}, 1 + \frac{w+a+b}{2}, \frac{D+w+a+b}{2} | \frac{1}{z} \right) \\
& \quad + (a \to -a) + (b \to -b) + (a \to -a, b \to -b),
\end{align*}
\]

and

\[
\begin{align*}
\text{DK}_2 &= \frac{1}{2\pi i} \text{Disc} i \int_M d^D x e^{i q \cdot x} x^\mu x^\nu \sqrt{-x^2} \ K_a(m\sqrt{-x^2}) K_b(m\sqrt{-x^2}) \\
&= -2^{a-b-3} \pi^{D/2} m^{-D-w-z} \frac{\Gamma(-a)\Gamma(-b)}{\Gamma(1-D-w+a+b+2)\Gamma(-w+a+b+2)} \\
& \quad \times 4F3 \left( \frac{1+a+b}{2}, 1 + \frac{a+b}{2}, \frac{w+a+b}{2}, \frac{D+w+a+b}{2} | \frac{1}{z} \right) \\
& \quad + (a \to -a) + (b \to -b) + (a \to -a, b \to -b).
\end{align*}
\]

Note that the factor \((-g^{\mu\nu})\) is omitted here for the sake of simplicity. These two functions \(\text{DK}_0(D, w, a, b, m, z)\) and \(\text{DK}_2(D, w, a, b, m, z)\) can be well regularized by an unorthodox regularization scheme: \(D = 4, a = a_0 + \alpha c\) and \(b = b_0 + \beta c\), with \(\alpha \neq 0, \beta \neq 0\) and \(\alpha \pm \beta \neq 0\). It is preferable to use irrational \(\alpha\) and \(\beta\) for practical calculation.

Accordingly, it is easy to write out the spectral density from \(\text{DK}_0(D, w, a, b, m, z)\) and \(\text{DK}_2(D, w, a, b, m, z)\). It is better to show the utility of this algorithm by a concrete example. From (39), one can write out the spectral density

\[
\rho^\text{pert}(z, c) = \frac{3m^4}{\pi^8} \left\{ \text{DK}_0(D, w, a, b, m_c, z) - 2 \text{DK}_2(D, w, a, b, m_c, z) \right\}
\]

with \(D = 4, w = -8, a = -2 + \epsilon\) and \(b = -2 + 3\epsilon\). Due to the \(\Gamma(-n + \alpha c)\) terms, a high precision computation is needed to get rid of roundoff errors. Fortunately, the hypergeometric function can be evaluated to arbitrary numerical precision by computation systems like the Python library \texttt{mpmath} [55] or Mathematica. Specifically, some numerical results are listed in Table 1. Note that the charm quark mass \(m_c\) is set to 1, and the working precision is set to 32 digits for \(\epsilon = 10^{-8}\). The exact value of \(\rho^\text{pert}(z)\) can be evaluate by using (42) or (46).

**Table 1:** Numerical evaluation of spectral density \(\rho^\text{pert}(z)\) with \(m_c = 1\).

| \(z\) | \(\epsilon = 10^{-4}\) | \(\epsilon = 10^{-6}\) | \(\epsilon = 10^{-8}\) | \text{Exact} |
|-------|----------------|----------------|----------------|----------------|
| \(1.1 \times 10^{-13}\) | 3.847514018 | 3.484073813 | 3.790001592 | 1.489432452 | 3.687774818 |
| \(2 \times 10^{-7}\) | 3.847553295 | 3.484354676 | 3.790789489 | 1.489904972 | 3.689380738 |
| \(5 \times 10^{-4}\) | 3.847553688 | 3.484357485 | 3.790797370 | 1.489909698 | 3.689396801 |
| \(10 \times 10^{-2}\) | 3.847553692 | 3.484357513 | 3.790797449 | 1.489909746 | 3.689396963 |
| \(20 \times 10^{-1}\) | 3.847551418 | 3.484073813 | 3.790001592 | 1.489432452 | 3.687774818 |

From Table 1, it is easy to see that one can use a finite small parameter to regularize the spectral density and obtain the numerical result to a desired precision. Several different input values of \(\epsilon\)
parameter are used to show the numerical stability of the algorithm. As $\epsilon$ decreases to zero, the numerical result steadily approaches the exact value, yet more digits of working precision is needed. Therefore, it is preferable to use a fairly small $\epsilon$ to save the computation time.

The numerical method can also be applied to the calculations of more complicated hypergeometric functions.

6 Conclusion

In this paper, a systematic and easy-to-use method is developed to calculate directly the doubly heavy hadron spectral density in the coordinate space. The correlation function is expressed in terms of generalized hypergeometric functions, and then the spectral density is obtained through two independent approaches: the simple integral representation method and the $\epsilon$-expansion method, respectively. It is found that the spectral density of doubly heavy hadrons can be analytically expressed through commonly known functions. After that, a concrete calculation is performed to show that the spectral density of doubly heavy hadrons can be easily obtained by using the coordinate space method. This method can drastically simplify the QCD spectral sum rule calculation of the $\{ccX\}$ and $\{bbX\}$ systems.

An instructive numerical method is developed to evaluate the $\epsilon$-regularized spectral density directly. This method can also be applied to other calculations where expressions are in the form of regularized (hypergeometric) functions. In particular, the numerical computation can be used to handle problems that are beyond the reach of the analytic $\epsilon$-expansion method.

Since the spectral density is expressed in terms of simple functions, there is no noticeable errors from multi-dimensional numerical integrals. A Monte-Carlo based uncertainty analysis [43, 44] can be used to make realistic uncertainty estimates of the phenomenological parameters. Such analysis can quantitatively improve the predictive ability of QCD sum rules. Moreover, this method can also serve to be an important cross-check of the widely used momentum representation method.

Furthermore, for a hadron state with two different massive quarks, the correlation function can be expressed in the form of Appell $F_4$ functions of two variables, as is shown in A. This type of spectral density can be used to study the $B_c$-like $\{cbX\}$ structures [21, 25, 56]. It is of great worth to work out the spectral density from the Appell $F_4$ functions. The calculations will be more complicated because the Appell $F_4$ is intricate and not widely studied like the generalized hypergeometric functions $pF_q$.

The method can also be extended to $\{QQQX\}$ and $\{QQ'X\}$ systems. These issues will be discussed in detail in a future publication.

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A Two massive quarks with different masses

In the case of two heavy quarks with different masses, one can also use the method of brackets [30–33] to calculate the integral of Bessel functions. Explicitly, this type of integral can be expressed in the
form of Appell $F_4$.

$$
\int_0^\infty dx \, x^{u-1} J_v(Qx) K_a(m_1x) K_b(m_2x)
= 2^{u-3} m_1^{-u-v+b} m_2^{-b} Q^v \frac{\Gamma(b) \Gamma(A_+ + \Gamma(A_-)}{\Gamma(1 + v)} F_4 \left( \frac{A_+ - A_-}{1 + v}, 1 - b \Big| \frac{-Q^2}{m_1^2}, \frac{m_2^2}{m_1^2} \right) + (b \rightarrow -b).
$$

(A56)

Appell $F_4$ is defined as

$$
F_4 \left( \begin{array}{c} \alpha; \beta \cr \gamma_1, \gamma_2 \end{array} \big| x, y \right) = \sum_{m,n=0}^{\infty} \frac{(\alpha)_{m+n}(\beta)_{m+n}}{m!n!(\gamma_1)_m(\gamma_2)_n} x^my^n.
$$

(A57)

The above integral can also be expressed as Appell $F_4$ with arguments $(-Q^2/m_1^2, m_2^2/m_1^2)$ or $(m_1^2/(-Q^2), m_2^2/(-Q^2))$. These three representations are related to each other by analytic continuation. If $m_1 = m_2 = m$, $F_4$ turns into $F_3$.

With the help of XSummer [57] and/or HYPERDIRE [42], $F_4$ may be reduced to commonly known functions and HPLs. If the analytic $\epsilon$-expansion procedure fails, one can use the method in Sec. 5 to evaluate the spectral density numerically.

References

[1] E. S. Swanson, “The New heavy mesons: A Status report,” Phys. Rept. 429 (2006) 243–305, arXiv:hep-ph/0601110.

[2] E. Klempt and A. Zaitsev, “Glueballs, Hybrids, Multiquarks. Experimental facts versus QCD inspired concepts,” Phys. Rept. 454 (2007) 1–202, arXiv:0708.4016 [hep-ph].

[3] N. Brambilla et al., “Heavy quarkonium: progress, puzzles, and opportunities,” Eur. Phys. J. C71 (2011) 1534, arXiv:1010.5827 [hep-ph].

[4] R. D. Matheus, S. Narison, M. Nielsen, and J. M. Richard, “Can the $X(3872)$ be a $1^{++}$ four-quark state?” Phys. Rev. D75 (2007) 014005, arXiv:hep-ph/0606297.

[5] F. S. Navarra, M. Nielsen, and S. H. Lee, “QCD sum rules study of $Q\bar{Q}-\bar{u}\bar{d}$ mesons,” Phys. Lett. B649 (2007) 166–172, arXiv:hep-ph/0703071 [hep-ph].

[6] R. D. Matheus, F. S. Navarra, M. Nielsen, and C. M. Zanetti, “QCD Sum Rules for the $X(3872)$ as a mixed molecule- charmonium state,” Phys. Rev. D80 (2009) 056002, arXiv:0907.2683 [hep-ph].

[7] S. Narison, F. S. Navarra, and M. Nielsen, “On the nature of the $X(3872)$ from QCD,” Phys. Rev. D83 (2011) 016004, arXiv:1006.4802 [hep-ph].

[8] Z.-G. Wang, “Mass spectrum of the scalar hidden charmed and bottomed tetraquark states,” Phys. Rev. D79 (2009) 094027, arXiv:0902.2062 [hep-ph].

[9] Z.-G. Wang, Y.-M. Xu, and H.-J. Wang, “Analysis of the scalar doubly heavy tetraquark states with QCD sum rules,” Commun. Theor. Phys. 55 (2011) 1049–1058, arXiv:1004.0484 [hep-ph].

[10] W. Chen and S.-L. Zhu, “The Vector and Axial-Vector Charmonium-like States,” Phys. Rev. D83 (2011) 034010, arXiv:1010.3397 [hep-ph].
[11] M.-L. Du, W. Chen, X.-L. Chen, and S.-L. Zhu, “The Possible $J^{PC} = 0^{+-}$ Exotic State,” arXiv:1203.5199 [hep-ph].

[12] R. Berg, D. Harnett, R. Kleiv, and T. Steele, “Mass Predictions for Pseudoscalar $J^{PC} = 0^{-+}$ Charmonium and Bottomonium Hybrids in QCD Sum-Rules,” Phys. Rev. D86 (2012) 034002, arXiv:1204.0049 [hep-ph].

[13] M. A. Shifman, A. I. Vainshtein, and V. I. Zakharov, “QCD and Resonance Physics. Sum Rules,” Nucl. Phys. B147 (1979) 385–447.

[14] M. A. Shifman, A. I. Vainshtein, and V. I. Zakharov, “QCD and Resonance Physics: Applications,” Nucl. Phys. B147 (1979) 448–518.

[15] L. J. Reinders, H. Rubinstein, and S. Yazaki, “Hadron Properties from QCD Sum Rules,” Phys. Rept. 127 (1985) 1.

[16] K.-C. Yang, W. Y. P. Hwang, E. M. Henley, and L. S. Kisslinger, “QCD sum rules and neutron proton mass difference,” Phys. Rev. D47 (1993) 3001–3012.

[17] L. Wang and F. X. Lee, “Octet baryon magnetic moments from QCD sum rules,” Phys. Rev. D78 (2008) 013003, arXiv:0804.1779 [hep-ph].

[18] H. Kim, S. H. Lee, and Y.-s. Oh, “Anti-charmed pentaquark $\Theta_c(3099)$ from QCD sum rules,” Phys. Lett. B595 (2004) 293–300, arXiv:hep-ph/0404170.

[19] S. Groote, J. G. Korner, and A. A. Pivovarov, “On the evaluation of a certain class of Feynman diagrams in x-space: Sunrise-type topologies at any loop order,” Annals Phys. 322 no. 10, (2007) 2374–2445, arXiv:hep-ph/0506286.

[20] M. Nielsen, F. S. Navarra, and S. H. Lee, “New Charmonium States in QCD Sum Rules: a Concise Review,” Phys. Rept. 497 (2010) 41–83, arXiv:0911.1958 [hep-ph].

[21] J.-R. Zhang and M.-Q. Huang, “$\{\bar{q}\bar{q}\} \{\bar{Q}(\prime)q\}$ molecular states,” Phys. Rev. D80 (2009) 056004, arXiv:0906.0090 [hep-ph].

[22] J.-R. Zhang, M. Zhong, and M.-Q. Huang, “Could $Z_b(10610)$ be a $B^*\bar{B}$ molecular state?,” Phys. Lett. B704 (2011) 312–315, arXiv:1105.5472 [hep-ph].

[23] W. Chen and S.-L. Zhu, “Possible $J^{PC} = 0^{+-}$ Charmonium-like State,” Phys. Rev. D81 (2010) 105018, arXiv:1003.3721 [hep-ph].

[24] Z.-G. Wang, “Analysis of the nonet scalar mesons as tetraquark states with new QCD sum rules,” Int. J. Theor. Phys. 51 (2012) 507–517, arXiv:1008.0974 [hep-ph].

[25] R. M. Albuquerque, X. Liu, and M. Nielsen, “Exotic $B_c$-like molecules in QCD Sum Rules,” arXiv:1203.6569 [hep-ph].

[26] J.-R. Zhang and M.-Q. Huang, “Heavy baryon spectroscopy in QCD,” Phys. Rev. D78 (2008) 094015, arXiv:0811.3266 [hep-ph].

[27] A. T. Suzuki and A. G. M. Schmidt, “Two-loop self-energy diagrams worked out with NDIM,” Eur. Phys. J. C5 (1998) 175–179, arXiv:hep-th/9709144.

[28] A. T. Suzuki and A. G. M. Schmidt, “Negative-dimensional integration revisited,” J. Phys. A31 (1998) 8023–8039.
[29] C. Anastasiou, E. W. N. Glover, and C. Oleari, “Scalar One-Loop Integrals using the Negative-Dimension Approach,” Nucl. Phys. B572 (2000) 307–360, arXiv:hep-ph/9907494.

[30] I. Gonzalez and I. Schmidt, “Optimized Negative Dimensional Integration Method (NDIM) and multiloop Feynman diagram calculation,” Nucl. Phys. B769 (2007) 124–173, arXiv:hep-th/0702218.

[31] I. Gonzalez and V. H. Moll, “Definite integrals by the method of brackets. Part 1,” arXiv:0812.3356 [math-ph].

[32] I. Gonzalez, V. Moll, and I. Schmidt, “A generalized Ramanujan Master Theorem applied to the evaluation of Feynman diagrams,” arXiv:1103.0588 [math-ph].

[33] I. Gonzalez, V. H. Moll, and A. Straub, “The Method of brackets. Part 2. Examples and applications,” arXiv:1004.2062 [math-ph].

[34] D. J. Broadhurst, J. Fleischer, and O. Tarasov, “Two loop two point functions with masses: Asymptotic expansions and Taylor series, in any dimension,” Z.Phys. C60 (1993) 287–302, arXiv:hep-ph/9304303 [hep-ph].

[35] D. Greynat, P. Masjuan, and S. Peris, “Analytic Reconstruction of heavy-quark two-point functions at O(αs3),” Phys.Rev. D85 (2012) 054008, arXiv:1104.3425 [hep-ph].

[36] S. Moch, P. Uwer, and S. Weinzierl, “Nested sums, expansion of transcendental functions and multi-scale multi-loop integrals,” J. Math. Phys. 43 (2002) 3363–3386, arXiv:hep-ph/0110083.

[37] S. Weinzierl, “Symbolic Expansion of Transcendental Functions,” Comput. Phys. Commun. 145 (2002) 357–370, arXiv:math-ph/0201011.

[38] T. Huber and D. Maitre, “HypExp, a Mathematica package for expanding hypergeometric functions around integer-valued parameters,” Comput. Phys. Commun. 175 (2006) 122–144, arXiv:hep-ph/0507094.

[39] T. Huber and D. Maitre, “HypExp 2, Expanding Hypergeometric Functions about Half-Integer Parameters,” Comput. Phys. Commun. 178 (2008) 755–776, arXiv:0708.2443 [hep-ph].

[40] M. Y. Kalmykov, B. F. L. Ward, and S. Yost, “All order epsilon-expansion of Gauss hypergeometric functions with integer and half/integer values of parameters,” JHEP 02 (2007) 040, arXiv:hep-th/0612240.

[41] M. Y. Kalmykov, B. F. L. Ward, and S. A. Yost, “On the all-order epsilon-expansion of generalized hypergeometric functions with integer values of parameters,” JHEP 11 (2007) 009, arXiv:0708.0803 [hep-th].

[42] V. V. Bytev, M. Y. Kalmykov, and B. A. Kniehl, “HYPERDIRE: HYPERgeometric functions Differential REDuction MATHEMATICA based packages for differential reduction of generalized hypergeometric functions: Now with $pF_{p-1}$, $F_1, F_2, F_3, F_4$,” arXiv:1105.3565 [math-ph].

[43] D. B. Leinweber, “QCD sum rules for skeptics,” Annals Phys. 254 (1997) 328–396, arXiv:nucl-th/9510051.

[44] L. Wang and F. X. Lee, “MathQCDSR: A mathematica package for QCD sum rules calculations,” Comput. Phys. Commun. 182 (2011) 1721–1731.

[45] R. Mertig, M. Bohm, and A. Denner, “FEYN CALC: Computer algebraic calculation of Feynman amplitudes,” Comput.Phys.Commun. 64 (1991) 345–359.
[46] A. I. Davydychev and M. Y. Kalmykov, “Massive Feynman diagrams and inverse binomial sums,” *Nucl. Phys.* **B699** (2004) 3–64, arXiv:hep-th/0303162.

[47] C. Anastasiou, K. Melnikov, and F. Petriello, “A New method for real radiation at NNLO,” *Phys.Rev.* **D69** (2004) 076010, arXiv:hep-ph/0311311 [hep-ph].

[48] J. Carter and G. Heinrich, “SecDec: A general program for sector decomposition,” *Comput.Phys.Commun.* **182** (2011) 1566–1581, arXiv:1011.5493 [hep-ph].

[49] E. Remiddi and J. A. M. Vermaseren, “Harmonic polylogarithms,” *Int. J. Mod. Phys.* **A15** (2000) 725–754, arXiv:hep-ph/9905237.

[50] D. Maitre, “HPL, a Mathematica implementation of the harmonic polylogarithms,” *Comput. Phys. Commun.* **174** (2006) 222–240, arXiv:hep-ph/0507152.

[51] D. Maitre, “Extension of HPL to complex arguments,” *Comput. Phys. Commun.* **183** (2012) 846, arXiv:hep-ph/0703052 [HEP-PH].

[52] W. Bühring, “Generalized hypergeometric functions at unit argument,” *Proc. Amer. Math. Soc.* **114** (1992) 145–153.

[53] W. Bühring, “Partial sums of hypergeometric series of unit argument,” *Proc. Amer. Math. Soc.* **132** (2003) 407–415, math/0311126. http://www.jstor.org/stable/1194069.

[54] S. Groote, J. G. Korner, and A. A. Pivovarov, “A new technique for computing the spectral density of sunset-type diagrams: Integral transformation in configuration space,” *Phys. Lett.* **B443** (1998) 269–275, arXiv:hep-ph/9805224.

[55] F. Johansson et al., *mpmath: a Python library for arbitrary-precision floating-point arithmetic (version 0.17)*, 2012. http://code.google.com/p/mpmath/.

[56] Z.-G. Wang, “Analysis of the vector and axialvector $B_c$ mesons with QCD sum rules,” arXiv:1203.6252 [hep-ph].

[57] S. Moch and P. Uwer, “XSummer: Transcendental functions and symbolic summation in Form,” *Comput. Phys. Commun.* **174** (2006) 759–770, arXiv:math-ph/0508008.