QCD SUM-RULE STUDY OF SCALAR MESONS

A Thesis Submitted to the College of Graduate Studies and Research in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy in the Department of Physics & Engineering Physics University of Saskatchewan - Saskatoon

By
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ABSTRACT

In this thesis, QCD Laplace sum-rules for the light quark $qq$ currents are employed to study the properties of the non-strange $I = 0$ and $I = 1$ light quark scalar mesons. This QCD sum-rule analysis allows us to interpret the experimentally observed $I = 0$ and $I = 1$ scalar mesons. The Hölder inequality technique is employed to determine the region of validity for the QCD sum-rule, and a stability analysis of the QCD sum-rule prediction is conducted through a Monte-Carlo uncertainty simulation of uncertainties.

The field theoretical content of the QCD sum rules incorporates purely-perturbative QCD contributions to two-loop order, leading contributions from QCD-vacuum condensates, and the direct single-instanton contributions in the instanton-liquid QCD vacuum model. Single-instanton contributions are the only components of the QCD field theory that distinguish between isospin states, and therefore they are responsible for breaking the mass degeneracy between the lowest-lying isovector and isoscalar mesons. A novel treatment of instanton effects in QCD continuum contribution is included in this thesis. There is also a need to go beyond the narrow resonance approximation for the scalar channels which are likely to exhibit sensitivity to broad resonance structure. A finite-width effect anticipated from physical resonance widths is incorporated for the hadronic content of the $I = 0$ and $I = 1$ QCD sum rules.

In the $I = 0$ channel, our results support interpretation of the $f_0(980)$ as the lowest-lying light quark scalar meson, indicating that $f_0(400 - 1200)$ is unnaturally decoupled from a light quark non-strange current. In the $I = 1$ channel, the results identify $a_0(1450)$ as the lowest-lying $qar{q}$ resonance, and are indicative of a non-$qar{q}$ interpretation for $a_0(980)$.
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DEDICATION

This thesis is dedicated to the memory of my grandmother Zhicai Qiu.
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Chapter 1

Foundations of Quantum Chromodynamics

1.1 Historical Review

There are, in principle, four kinds of fundamental forces (interactions) existing in nature to our present knowledge: gravitation, electromagnetism (EM), weak interaction and strong interaction.

Gravitation is described classically by the general theory of relativity. It is believed that this interaction proceeds by exchange of Gravitons, and is currently believed to play a negligible role in elementary particle physics on the phenomenological level.

Electromagnetic interactions (e.g. Coulomb scattering) are carried by the massless spin-one photons. There is only one kind of photon, and they do not interact among themselves. EM interaction can be best described by Quantum electrodynamics (QED) which was formulated in about 1950 [1].

After EM and gravitation, the remaining strong and weak interactions in nature are associated with nucleons. Weak interactions (e.g. β-decay, μ-decay) describe forces between nucleons which involve leptons (i.e. e, μ). In weak interactions, W⁺, W⁻ (≈ 80 GeV) and Z⁰ (≈ 91 GeV) carry the forces. Thanks to the pioneering work of Glashow, Weinberg and Salam [2, 3], we now know that the weak and EM interactions are connected closely and can be described by a single theory of electroweak interactions.

The remaining strong interaction is the main concern in this thesis, and will be described in much more detail.

The strong interaction describes forces which act among hadrons such as
protons, neutrons, pions, kaons, etc.

In 1935, Yukawa developed a theory that attempted to describe the strong interaction [4]. In his theory, the pion is the carrier of the nucleon forces. Although it is relatively successful, especially the discovery of \( \pi^- \) in 1947 [5], the Yukawa theory met several difficulties:

1. At high energies, the proton-neutron forces were not well described by pion exchange.

2. Due to parity, the interaction between pions could not be described by pion exchange.

3. This theory is non-renormalizable and hence has limited predictive power.

A better theory is obviously needed to describe strong interactions. To date, Quantum Chromodynamics (QCD) is widely accepted as the correct theory for the strong interaction. In the following, a brief review of the historical development of QCD is given.

First let's ask the question: are the neutrons and protons fundamental spin-\( \frac{1}{2} \) particles? If they are not, what are they made up of? The best evidence for substructure first comes from \( e^- p \) deep inelastic scattering and the parton model, which was introduced at the end of 1960s by Feynman [6], Bjorken [7] and others. Deep inelastic scattering happens when a very high energy electron scatters with a proton. The proton breaks up into an arbitrary number of hadron states, and the invariant mass of the hadrons in the final state must be at least as large as the mass of the proton. Experimental evidence shows that the proton has substructures at distances less than 1 fm.

The famous result from deep inelastic scattering is known as Bjorken scaling [7]. Let us define the 4-momentum \( q^2 \) transferred in the system, \( \mu \) the energy loss of electron, and \( \omega = \frac{2M\mu}{q^2} \) a dimensionless variable. The Bjorken scaling
says that at high $\mu$ and $q^2$, but moderate $w$, the structure functions $W_1$ and $\mu W_2$ turn out to be functions of $w$ only, not of $q^2$ and $\mu$ separately. Feynman interpreted this phenomenon by the parton model [6], which describes rapidly moving hadron (e.g. the proton) as equivalent to a jet of free particles called partons. So in deep inelastic scattering, electrons scatter, not from the whole proton, but incoherently from its point-like free constituents (partons). After accepting the parton structure of hadrons, it is easy to determine the spin $1/2$ of the parton by measuring the value of $[(\frac{2W_2}{q^2}) W_2 - W_1]/(2W_1)$.

Even before the discovery of the parton model, during the 1950's and 1960's, due to the contribution of the discovery of "resonances", a hadronic population explosion was observed amongst strongly interacting particles. and hundreds of hadrons were known. The classification of different hadrons was a big challenge at that time. The decisive breakthrough in this respect was made by Gell-Mann and by Ne'eman in 1961 [8, 9]. When plotting certain then-known hadrons on a isospin-hypercharge ($I - Y^-$) plane, regular patterns always occurred. The existence of these patterns suggested that hadrons are composite states of more fundamental entities known as "quarks". At that time, they suggested three fundamental spin-$1/2$ quarks which were denoted as $u, d, s$ quarks. Only the $s$ quark carries the strangeness quantum number. They designed a scheme for classifying all the then-known hadrons according to the representations of the flavour SU(3) group. Nowadays, there are believed to be six quarks distinguished by $u, d, s, c, t, b$, the other three flavours being substantially more massive than the (light) $u, d, s$ quarks.

According to the quark model, all hadrons can be classified into two groups: baryons and mesons. Baryons are fermionic bound states of three quarks ($qqq$), and mesons are bosonic quark-antiquark pair ($\bar{q}q$) states. All quarks are spin $1/2$ and carry non-integer electric charges. The quark model was soon accepted
as the correct theory to describe hadronic states, and physicists identified the parton as the quark.

In summary, the parton model served as the dynamical evidence for the existence of quarks.

- A rapidly moving hadron of momentum $p$ is equivalent to a jet of free particles called partons. Partons travel parallel to the original hadron, sharing its momentum.

- Reaction rates for hadrons are obtained from incoherent parton reaction rates.

- Probability of having a parton of momentum $\zeta p$ is $N(\zeta)d\zeta$.

Very soon it was realized that the quark model, if taken seriously, posed a further puzzle. Let us consider the $\Delta^{++}$, for example. This particle is made up of three $u$ quarks ($uuu$). The three $u$ quarks are all in $S = \frac{1}{2}$, $L = 0$ states, and the symmetric spatial wave function has made the three quarks all in parallel spin states, which obviously violates Fermi-Dirac statistics. To solve this puzzle, in 1973, Fritzsch and Gell-Mann assigned the quark a new degree of freedom [10], called colour. With the help of the colour degree of freedom, it is easy to construct a totally antisymmetric wave function correctly describing the $\Delta^{++}$.

How many colour-degrees of freedom are in the theory? The ratio of cross sections for $e^-e^-$ scattering producing hadrons (inclusive process) to that of producing muons. $R = \frac{\sigma(e^-e^-\rightarrow\text{hadrons})}{\sigma(e^-e^-\rightarrow\mu^+\mu^-)}$, indicates there are 3 colours (red, green, blue) existing in nature.

So far, with the help of three flavour and three colour degrees of freedom, the parton-quark model had proved to be very efficient in qualitatively describing
the spectrum and static properties of mesons and baryons. For a complete strong interaction theory, the dynamical side of the theory is needed.

The search for quark dynamics was initiated right after the foundation of the parton model. All the known quantum field theories at that time were surveyed as possible candidates for quark dynamics. and were shown not to solve the following properties of the quark interaction:

- When the distances probed are very small \(\text{i.e.},\) when the momentum transferred by the probe was very high, the situation occurring in deep inelastic scattering, the force between quarks is surprisingly weak and the quarks move rather like free particles.

- On the other hand, no free quarks have ever been observed, so it is sure that over large distances, the force between quarks becomes increasingly strong, leading to the phenomenon known as quark confinement.

This situation changed after the breakthrough discovery of asymptotic freedom [11, 12, 13] after the classical work of Yang and Mills [14]. This theory is a gauge theory similar to quantum electrodynamics though different from it in that the corresponding gauge symmetry is not Abelian \(\text{i.e.}\) the generators of the symmetry group are non-commutative. Gross \textit{et al.} examined non-Abelian gauge field theories by the use of the renormalization group method (as will be discussed later), and found these field theories satisfied the desired property, which is now called asymptotic freedom: the strong coupling constant is strong at large distance while weak at short distance. Soon after it was shown that only non-Abelian gauge theories exhibit the property of asymptotic freedom among the known theories in four dimensional space-time [15].

Combining the quark model and the asymptotic freedom property of the non-Abelian gauge theory together, we have reached the celebrated quark dy-
namical theory Quantum Chromodynamics (QCD). The term “chromo” refers to the colour symmetry of the quark system. There are various reasons for believing that QCD is the best theory of strong interaction.

Just like the photon, which is an Abelian gauge field mediating EM interaction between charged particles in QED, the non-Abelian gauge field of QCD mediates colour interactions between quarks. This non-Abelian gauge field in QCD is called the gluon as it is responsible for binding quarks together. While photons have no electric charge, gluons carry colour charges and hence they can interact with each other in the absence of quarks. This property of the gluon is an essential ingredient for having asymptotic freedom.

In the quark model with colour symmetry $SU(3)_c$, hadrons appear as colourless states while quarks carry colour quantum numbers. It is assumed that only colourless states are physically realized and hence quarks cannot be observed in isolated states. This also is the reason why only meson ($\bar{q}q$) and baryon ($qqq$) states can be observed in nature, because these combinations of quarks and antiquarks can form colour-singlet states.

According to the property of asymptotic freedom of QCD, one can safely use perturbation theory to calculate short-distance (large energy) reactions. On the other hand, when distances become large in reactions, the effective coupling constant grows large correspondingly, and perturbative QCD loses its power in this region. In the long-distance (low energy) region, non-perturbative QCD has to be applied to make QCD a complete theory. QCD sum rules, instantons, and lattice-gauge theory are some examples of non-perturbative QCD. In this thesis, the first two of these non-perturbative QCD methods will be presented.
1.2 Principles of Perturbative QCD

1.2.1 Gauge Principles

As discussed in the last section, QCD is a quantized non-Abelian gauge field theory. We start with an elementary introduction to gauge field theories based on gauge principles and then describe the methods of quantizing gauge field theories.

Gauge field theories are field theories based on gauge principles. In general, gauge symmetries can be either abelian or nonabelian, and are realized either locally or globally.

Before discussing the various gauge symmetries, a brief discussion of the Lagrangian formulation of the field theory, which plays a central role in the contemporary understanding of interactions and symmetries, is helpful. In brief, the Lagrangian satisfies five requirements:

1. **Lorentz invariance**, which means that Lagrangian $\mathcal{L}$ must be a scalar with appropriate dimensions under Lorentz transformation.

2. **Gauge invariance**, which means that field theories satisfy certain gauge symmetry requirements.

3. **Locality**, which means that $\mathcal{L}$ depends on local properties of fields, i.e., $\mathcal{L}$ depends on fields $\phi(x)$ and a finite number of derivatives. Usually, only the first derivative of the field $\partial_\mu \phi(x)$ is used in Lagrangian formulation.

4. **Renormalizability**, which is the ability to absorb the divergences into the original Lagrangian. This is the key difficulty in constructing the theory.

5. **Unitarity**, which means that the $S$ matrix (can be obtained from Lagrangian) satisfies the unitary requirement $S^\dagger S = 1$. 

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In the content of classical physics, by “Lagrangian formulation” we mean “the principle of least action”. The action $S$ is defined as

$$S[\phi] = \int d^4x L(\phi(x), \partial_\mu \phi(x))$$

(1.1)

The least action principle says fields which actually occur in nature correspond to the shortest path in the space-time, or a stationary value of the action $\delta S[\phi] = 0$. This gives us a dynamical principle on which we base our formulation of the problem. The least action principle leads to the well known Euler-Lagrange equation (i.e. the equation of motion) for the field $\phi(x)$ analogous to Newton’s equation of motion for point masses.

$$\frac{\partial L}{\partial \phi} - \frac{\partial}{\partial x^\mu} \left( \frac{\partial L}{\partial (\partial_\mu \phi)} \right) = 0$$

(1.2)

Now we have the background to discuss the gauge symmetry of the Lagrangian. Let’s start from the easiest one.

1. **Global – Abelian gauge invariance** *(e.g. charge conservation)*

Global means the symmetry operations do not involve space-time. Abelian means that different transformations of the group commute with each other. One example of a global-Abelian transformation is the phase transformation $\phi_j(x) \rightarrow \phi'_j(x) = e^{-i q_j \theta} \phi_j(x)$, where $\theta$ is a real number and independent of space-time $x$. The phase $\theta$ is not measurable and thus can be chosen arbitrarily, but once chosen it must be the same for all spacetime.

When $\theta$ becomes infinitesimal, $\delta \phi_j(x) = \phi'_j(x) - \phi_j(x) = -i q_j \theta \phi_j(x)$. The global invariance requires $\delta L \equiv 0$, and with the help of the Euler-Lagrange equation (1.2), one finds that any continuous symmetry transformation which leaves the Lagrangian $L$ invariant implies the existence
of a conserved quantity, a statement of Noether’s Theorem. In our case, the conserved quantity is the conserved current $J^\mu = \eta_{\mu \nu} \frac{\delta \mathcal{L}}{\delta \partial_\nu \phi}$ where the charge is defined by $Q = \int d^3x J_0(x)$. The charge defined in this way is a constant of motion $\frac{dQ}{dt} = 0$ because the surface terms at infinity become negligibly small $\int d^3x \partial_\nu J_0 = \int d^3x \partial^\mu J_\mu = 0$. Noether’s theorem is the connection between symmetries and conservation laws in field theories.

2. Global non-Abelian gauge invariance (e.g., isospin symmetry)

The generalization to non-Abelian transformations is fairly simple in the global case. The simplest non-Abelian invariance is isospin where the fields are assumed to come in multiplets. The multiplets are defined as $\phi = (\phi_1, \phi_2, \phi_3)$, forming a basis for representations of the isospin group SU(2) involving rotations in isospin space. The gauge transformation is specified by three parameters in SU(2), $\theta = (\theta_1, \theta_2, \theta_3)$, the transformation is defined as $\phi \rightarrow \phi' = e^{-i\tilde{L}\theta_\phi}$. where $\tilde{L}$ is a matrix denoting the generators of SU(2) transformations. The algebra satisfied by the generators $\tilde{L}$ is $[L^i, L^k] = i\epsilon^{ijk} L_i$, where the $\epsilon^{ijk}$ are called the structure constants of the group and are antisymmetric under exchange of any pair of indices. For an infinitesimal transformation, $\delta \phi = \phi - \phi' = -i\tilde{L} \cdot \theta \phi$, which makes the Lagrangian invariant under this global gauge transformation.

3. Local – Abelian gauge invariance (QED)

Consider a transformation $\phi_j(x) \rightarrow \phi'_j(x) = e^{-iq_j \theta(x)} \phi_j(x)$. where $\theta(x)$ is an arbitrary function of $x$. The local gauge transformation means that one can measure and fix the phase $\theta(x)$ locally and differently at different points in space-time. The infinitesimal transformation is $\delta \phi_j(x) = -iq_j \theta(x) \phi_j(x)$. The difference occurs when differentiating the
field term, $\partial_\mu \phi_j(x) \not\to e^{-ie_0 A(x)} \partial_\mu \phi(x)$, which is an inherent requirement of the Lagrangian to be invariant under gauge transformation. EM interaction is said to be locally invariant because all derivatives can be replaced by “covariant derivatives” $D_\mu \equiv \partial_\mu - ieq_j A_\mu$. By this replacement, one can rebuild the required properties $D_\mu \phi_j(x) \not\to e^{-ie_0 A(x)} D_\mu \phi_j(x)$. Thus the gauge invariance of the Lagrangian follows as it did in the global case.

In QED, $A_\mu(x)$ is the vector potential of the photon, the simplest example of a “gauge field”. The vector potential transforms as $A_\mu(x) \to A'_\mu(x) \equiv A_\mu(x) - \frac{ie}{c} \frac{\partial_\mu \phi_j(x)}{\partial x^\nu}$, where the potential is associated with the massless photon and $e$ is the unit EM charge. The “field strength tensor” $F_{\mu\nu}$ is defined as $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, which is itself invariant under local Abelian gauge transformation. Therefore the photon kinetic energy is gauge invariant if constructed with the field strength tensor $F_{\mu\nu}$. In QED, the Lagrangian can be written as $\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu}$.

4. Localnon-Abelian gauge invariance (QCD)

The first generalization of SU(2) to a locally gauge invariant Lagrangian is due to Yang and Mills [14]. In the Yang-Mills case, the $SU(N)$ group generators $T_j$ obey $[T_j, T_k] = ie^{jk} T_i$, which is the same as the global non-Abelian case. The field multiplet is defined as $\psi = (\psi_1, \psi_2, \cdots, \psi_N)$. The aim here is to introduce as many vector fields $A_\mu^j(x)$, gauge fields that are analogous to the photon field $A_\mu$ in QED, as is necessary in order to construct a Lagrangian invariant under the local gauge transformation specified by $\theta_j(x)$. By analogy with QED, we seek a “covariant derivative” $D_\mu$ instead of the ordinary derivative $\partial_\mu$, such that $D_\mu \psi(x) \to D'_\mu \psi(x) = e^{-iA_\mu(x)} D_\mu \psi(x)$. The following definition of $D_\mu$
satisfies the above requirement. \( D_\mu = \partial_\mu - ig \vec{T} \cdot A_\mu \), where \( g \) is the coupling constant. Similar to QED, a generalized field tensor is defined as 
\[ F^{\mu \nu}_{\mu \nu} = \partial_\mu A^\nu_\nu - \partial_\nu A^\mu_\mu + gc_{ijkl} A^k_\mu A^l_\nu, \]
and \( F^i_{\mu \nu} F^j_{\mu \nu} \) is gauge invariant. Thus a gauge invariant Lagrangian can be constructed as follows:
\[
\mathcal{L} = -\frac{1}{4} F_{\mu \nu}^i F^{i \mu \nu} + \bar{\psi} (i \gamma^\mu D_\mu - m) \psi. \tag{1.3}
\]

It should be noted that in the above equation, gauge invariance implies there exists only one interaction parameter \( g \), which can be determined by experiments.

After studying the four kinds of gauge symmetry cases, many similarities between QED (local Abelian case) and QCD (local non-Abelian case) have been found, including use of the covariant derivative to build gauge invariant field transformations. However, QCD and QED study totally different interactions, so it is worthy to highlight the essential differences between QCD and QED.

The self-coupling of the gauge bosons (gluons) accounts for the major difference between QCD and QED. Due to the quadratic term of the field term in field tensor \( F_{\mu \nu} (gf_{abc} A^a_\mu A^b_\nu) \), three and four \( A_\mu^a \) products terms are found in \( \mathcal{L} \), and these terms imply the 3 and 4 gluon interactions, as shown in Figure 1.1, which do not directly occur from photon interactions in QED. It is in fact these interactions of gluons themselves which are responsible for the property of Asymptotic Freedom of QCD.

1.2.2 Second Quantization

Second quantization is the quantization of gauge fields, especially the Yang and Mills' gauge field. Quantization is not at all a unique procedure and a variety of quantization methods may exist which lead to the same physical
prediction. Basically, there are two ways of quantization: the canonical operator formalism \cite{16} and the functional-integral formalism \cite{17}. In the traditional canonical operator formalism, one regards fields as operators and sets up canonical commutation relations for them. All Green's functions which characterize the quantum theory of fields may then be calculated as vacuum expectation values of the product of field operators. In the Feynman functional-integral (path integral) formalism, fields are c-numbers and the Lagrangians are of the classical form. Green's functions are determined by integrating the product of fields over all possible functional forms with a suitable weight. Comparing the two methods, we find three advantages of the path integral over the canonical operator formalism method:

1. As the classical form of the Lagrangian appears in the functional integral, this formalism is convenient for dealing with systems such as gauge symmetries obeyed by the classical Lagrangian.

2. Canonical quantization has difficulties in dealing with non-Abelian gauge field theories, which need the supplementary contributions of Faddeev-Popov ghost fields \cite{18, 19}.

3. The functional integral formalism is easier in dealing with the non-perturbative regime of QCD.
Because of the above three advantages, in this thesis, only Feynman's functional integral method will be employed in this thesis as the tool for second quantization of the non-Abelian gauge field in QCD.

In particle physics, one of the most used results of quantum mechanics is the prediction of cross-section of particular process. The cross-section depends on the Green's function $K$, which is the probability that a particle located at time $t_1$ and coordinate $x_i$ will be present at space-time $x_f, t_f$. $K(x_f, t_f, x_i, t_i) = \langle x_f t_f | x_i, t_i \rangle$. We further define the Green's function $G(t_1, t_2)$, which is necessary for $S$ matrix elements in quantum mechanics.

$$G(t_1, t_2) = \langle O | T(\hat{x}_1(t_1)\hat{x}_2(t_2)) | O \rangle \quad (1.1)$$

where $|O\rangle$ is the ground state, $T$ is the time product and $\hat{x}(t)$ is the Heisenberg position operator. Extension of these ideas to a quantum field theory leads to a functional integral representation for the Green's function of field operators [17]:

$$G(t_1, \cdots, t_n) = \langle 0 | T(\hat{\phi}(x_1) \cdots \hat{\phi}(x_n)) | 0 \rangle = \frac{\int [d\phi]\phi_1 \cdots \phi_n e^{iS}}{\int [d\phi] e^{iS}} \quad (1.5)$$

where $S$ is the classical action $S = \int d^4L$ and $[d\phi]$ means the integration over all possible field configurations at every space-time point $(x, t)$.

After establishing the above relation, one can calculate any Green's function in the functional integral formalism without reference to the operator language. Furthermore, the above equation can be rewritten in a more compact form by using the concept of functional derivative with respect to an external source first introduced by Schwinger [20].

Let us consider an external source function $J(x)$ and introduce an artificial source term $\phi(x)J(x)$ in the functional integral which gives the generating
function $Z[J]$:

$$Z[J] = \frac{1}{N} \int [d\phi] \exp \{i \int d^4 x (\mathcal{L} + \phi J)\}$$

(1.6)

$N$ is the normalization constant which is independent of $J(x)$. The functional differentiation is defined as.

$$\frac{\delta Z[J(x)]}{\delta J(y)} = \lim_{\epsilon \to 0} \frac{Z[J(x) - \epsilon \delta(x - y)] - Z[J(y)]}{\epsilon}$$

(1.7)

According to the definition, we have

$$G(t_1 \cdots t_n) = \langle 0 | T(\phi(x_1) \cdots \phi(x_n)) | 0 \rangle = \frac{\delta}{i \delta J(x_1)} \cdots \frac{\delta}{i \delta J(x_n)} Z[J] \bigg|_{J=0}$$

(1.8)

The physical interpretation of the generating function is the vacuum to vacuum transition amplitude in the presence of the source $J$. $Z[J] \equiv \langle 0 | J | 0 \rangle$. The normalization factor $\frac{1}{N}$ guarantees $Z[0] = 1$.

Now Feynman's path integral method can be applied to the non-Abelian gauge field theory (QCD). In order to provide the unitarity in the physical space of states, ghost-fields $\omega(x)$, which are scalars satisfying Fermion statistics, are introduced in the original Lagrangian (1.3). A mathematical tool to describe the fermion fields (ghosts and quarks) is known as Grassmann Algebra [21].

In order to obtain the propagator for the gauge fields, one should introduce the gauge-fixing term. The procedure given by Faddeev and Popov allows one to include any gauge-fixing term in the Lagrangian [19]. Because of the introduction of the gauge-fixing term, the QCD Lagrangian is no longer gauge invariant. In order to rephrase gauge invariance, Becchi, Rouet and Stora introduced a non-linear transformation called BRS transformation which extends
gauge invariance to the ghost field and thus leaves the full QCD Lagrangian invariant [22].

In summary, to generate a Green's function for non-Abelian gauge theories, the anticommuting sources $\bar{J}^a_\omega, J^a_\omega$ for ghost fields $\omega_a, \bar{\omega}_a, \bar{\xi}_f, \xi_f, \bar{J}^a_q, J^a_q$ for quark fields $q^f, \bar{q}^f$ and commuting sources $J^a_\mu$ for the gluon $B^a_\mu$ are introduced. We write the final form of the functional as:

$$Z[\eta, \bar{\eta}; \bar{\xi}, \xi; \lambda] = \int [dq][d\bar{q}][d\omega][d\bar{\omega}][dB]\exp\{i \int d^4x (\mathcal{L}_{QCD} + \mathcal{L}_{source})\}$$

(1.9)

$$\mathcal{L}_{QCD} = \sum_q \{i\bar{q} D \cdot q - m_q \bar{q}q\} - \frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} - \frac{1}{2\xi} (\partial \cdot B)^2 - \sum_{a,b,c} (\partial_{\mu}\omega_a)(\partial_{\nu}B^a_{\mu}) - \sum_{a,b} B^a_{\mu} B^a_{-\mu}$$

(1.10)

where $\xi$ is the gauge parameter and

$$\mathcal{L}_{source} = \sum \{ \bar{J}^a_\omega \omega_a + \bar{\omega}_a J^a_\omega + \bar{J}^a_q q^f + q^f J^a_q - J^a_{au} B^a_\mu \}$$

(1.11)

1.2.3 Regularization and Renormalization

The key difficulty in QCD is renormalization. With the Lagrangian for QCD (1.10), the Feynman rules for QCD can be established. Given any quantum field theory, one can construct the Feynman rules for calculating the Green's function and $S$-matrix elements in perturbation theory, which in turn gives the cross section for an arbitrary quark-gluon process. It will be seen later that the lowest-order calculation in a quark-gluon process generally reproduces the parton-model results. Thus the parton picture corresponds to the tree level (i.e. no loop diagram) in the perturbative expression based on the QCD Lagrangian (1.10).
Figure 1.2: One-loop quark self-energy $\Sigma(p)$.

In the tree approximation, however, dynamical effects of QCD do not show up and the really important ingredient of QCD is hidden in QCD radiative corrections to the tree amplitudes, which necessarily include the contributions of loop diagrams.

In general, the loop contribution to a Green's function generates infinities because the momentum variable in the loop integral ranges over an infinite range. In other words, for a relativistic theory, there is no intrinsic cut-off in momentum. For example, consider the one-loop diagram for the quark self-energy $\Sigma(p)$ in QCD. The Feynman diagram shows in Figure 1.2 leads to the following self-energy in the Feynman gauge ($\xi = 1$).

$$\sum(p) = g^2 C_f \int \frac{d^4k}{(2\pi)^4} \frac{\gamma_\mu (m+\frac{p-k}{|k|}) \gamma^\mu}{ik^2 (m^2 - (p-k)^2)} \quad (1.12)$$

By simple power counting in $k$, we have $\int d^4k \frac{k^2}{k^4} \sim k$ at the limit of $k \rightarrow \infty$, thus the divergence comes from the high-momentum region $|k| \rightarrow \infty$. These divergences will render the calculation formally meaningless. The theory of renormalization is a method that allows us to consistently isolate and remove all these infinities from the physically measurable quantities. The procedure which makes divergent integrals tentatively finite by introducing a suitable convergence device is called regularization. Regularization is a purely mathematical procedure and has no physical consequences (i.e. the regularization
procedure happens in the intermediate stage). Accordingly it is not a unique procedure, and a variety of schemes exist. The cut-off method and dimensional regularization (Dim-Reg) are two widely used schemes.

A cut-off is a simple regularization schemes where the high-momentum region, the source of the divergence, is cut-off in the divergent integrals. The method was improved in earlier literatures in QED [23]. It, however, breaks translation invariance and hence the shifting of momentum in the integral changes the results. Therefore, it is not suitable for the regularization of gauge theories.

Dim-Reg is a method which makes divergent multiple integrals convergent by reducing the number of multiple integrals. The basic idea behind this scheme is that since the divergences in Feynman diagram come from the integration of internal momentum in four-dimensional space, the integrals can be made finite by allowing the dimension of space-time [11, 24] These divergences will manifest themselves as singularities as the dimension goes to four. Hence, in Dim-Reg we keep the space-time dimension $D$ lower than 4 and replace the divergent 4 dimension integral by a $D$ dimensional integral. Since in Dim-Reg, nothing has been violated expect that space-time is not 4 dimensional, all physical requirements are satisfied. Therefore, this scheme is Lorentz invariant, gauge invariant, unitary, etc. [25]. In this sense Dim-Reg is the most suitable scheme for gauge theory, and it is employed as the regularization scheme in this thesis. Virtually all modern calculations are done in Dim-Reg.

Still using the above quark self-energy example (1.12), in Dim-Reg scheme, the integral form $\int \frac{d^4 k}{(2\pi)^4}$ is calculated in $D$ (continuous) dimensions instead of 4 dimensional space: the integral form is changed to $\mu^{1-D} \int \frac{d^D k}{(2\pi)^D}$. The arbitrary mass parameter $\mu$ is introduced to keep the coupling constant $g_0$ dimensionless in the Lagrangian (1.10). In the chiral limit ($m_q = 0$), the quark self-energy
has the following form [26]:

\[
\sum(p) = \frac{-g_0^2}{(4\pi)^2} C_F \not{p} \left( \frac{1}{\epsilon} - \gamma_E + 1 - \ln\left(\frac{-p^2}{4\pi \mu^2}\right) \right) + \mathcal{O}(\epsilon) \quad (1.13)
\]

where \( \epsilon = \frac{D-4}{2} \). \( \gamma_E \) is the Euler’s constant, and we restrict ourselves to the Feynman gauge \( \xi = 1 \). As the dimension \( D \) approaches 4, the divergence comes from the \( \frac{1}{\epsilon} \) term.

With the help of the dimensional regularization scheme and the above quark self-energy example, we can discuss the “renormalization”, which means, together with the redefinition of the field, mass and coupling constant, the readjustment of the normalization of the Green’s function by suitable multiplicative factors which may eliminate possible infinities in the Green’s function.

As an example, using the above quark self-energy example, the quark propagator in the massless quark case can be defined as:

\[
\tilde{S}_{ij}(p) = \frac{\delta_{ij}}{(m - \not{p} \sum(p))} = \frac{\delta_{ij}}{\not{p} \left( 1 + \sigma(p^2) \right)} \quad (1.14)
\]

where \( \sigma(p^2) \) is defined as

\[
\sigma(p^2) = \frac{-g_0^2}{(4\pi)^2} C_F \not{p} \left( \frac{1}{\epsilon} - \gamma_E + 1 - \ln\left(\frac{-p^2}{4\pi \mu^2}\right) \right) + \mathcal{O}(g_0^1) \quad (1.15)
\]

We can normalize the quark propagator \( \tilde{S}(p) \) by a multiplicative factor of \( Z_2 \) which corresponds to the quark field’s renormalization constant. The renormalized propagator \( \tilde{S}_{R,ij}(p) \) is defined as \( \tilde{S}_{R,ij}(p) = Z_2^{-1} \tilde{S}_{ij}(p) \). The quantity \( Z_2 \) can be expanded in power of \( g_0 \) (i.e. \( Z_2 = 1 - z_2 + \mathcal{O}(g_0^1) \)). The order \( g_0^2 \) term \( z_2 \) is assumed to be divergent. Thus,

\[
\tilde{S}_{R,ij}(p) = -\frac{\delta_{ij}}{\not{p} \left( 1 + \sigma(p^2) \right)} \frac{1}{z_2} \quad (1.16)
\]
We can choose the divergent term in \( z_2 \) to just cancel the divergent term in \( \sigma(p^2) \) which renormalizes the whole quark propagator (i.e. renders it finite in the \( \epsilon \to 0 \) limit).

Note here that the way of eliminating divergences in quantum theory is not unique because there exists an ambiguity in defining the divergent piece of the Green's function (different regularization methods lead to different divergences in Green's function), and thus there exists an ambiguity in choosing the way to render the divergent term finite (i.e. the arbitrariness of choosing the \( z_2 \) term in the propagator). In order to remove this ambiguity, one has to specify how to define the divergent term, which will be subtracted out in the renormalization process. The description of how to subtract divergences in Green functions is called a renormalization scheme. Two widely used such schemes are minimal subtraction (MS) and modified minimal subtraction (\( \overline{\text{MS}} \)).

1. MS is due to t' Hooft [27] and is specific to Dim-Reg. In the MS scheme, only the pole terms in the dimensionally regularized expression of the Green's function are eliminated. This is the most economical scheme and leads a simple expression for the renormalization constant, while the renormalized Green's function has a rather complicated form (in the MS scheme, the renormalization constant \( z_2 = -\frac{g^4}{(4\pi)^2} C_F \frac{1}{\epsilon} \)).

2. \( \overline{\text{MS}} \) eliminates the \( \{ \frac{1}{\epsilon} + \gamma_E - \ln(4\pi) \} \) term instead of only \( \frac{1}{\epsilon} \) term in the Green's function. It is frequently used in the definition of QCD coupling constant and also in other applications of gauge field theories because it leads a rather compact form for the renormalized Green's function. In the \( \overline{\text{MS}} \) scheme, \( z_2 = -\frac{g^4}{(4\pi)^2} C_F \{ \frac{1}{\epsilon} - \gamma_E + \ln(4\pi) \} \).

As seen from the above description, at each order of the perturbation theory, the removal of divergences turns out to be a subtraction of divergent pieces in
the proper Green's function. The central question of renormalization theory depends on whether the above subtraction process can be consistently performed to all orders with a finite number of multiplicative factors (i.e. the renormalization constants) and parameters which (such as $g$ and $m$) will be redefined. One can show that the renormalization procedures are successfully carried out in a restricted class of interactions. We use the power counting method to determine this particular class. Detailed techniques are outlined in [28].

After a certain $\mathcal{L}$ is determined renormalizable by power counting, for every distinct divergent term in the original $\mathcal{L}$, a counter term of the same structure multiplied by a constant is introduced. These counter terms serve as to cancel the divergences from the corresponding terms in the original $\mathcal{L}$ and to give a finite Green's function. It is worth noting that the above method of eliminating the divergences using counter terms is essentially the same as the multiplicative renormalization method given previously.

In summary, after a certain interaction is determined renormalizable by the power counting method, counter terms are introduced to cancel the divergences in the original $\mathcal{L}$. For QCD case, the renormalized Lagrangian $\mathcal{L}_R^{QCD}$ is:

$$
\mathcal{L}_R^{QCD} = - \frac{Z_{YM}}{2} \partial_{\mu} A_\mu^a (\partial_{\nu} A_\nu^a - \partial_{\nu} A_\mu^a) - \frac{Z_5}{2 \xi} (\partial_{\mu} A_\mu^a) (\partial_{\nu} A_\nu^a)
+ \frac{i Z_{2F} e}{\sqrt{\alpha}} \partial_{\nu} - Z_v m_L \phi_v - Z_{1F} g \phi \partial^\mu A^a \partial_\mu \phi
- \frac{Z_0}{2} g f_{abc} (\partial_{\mu} A_\mu^a - \partial_{\nu} A_\mu^a) A_\mu^b A_\mu^c
- \frac{Z_5}{4} g^2 f_{abc} f_{ade} A_\mu^a A_\nu^b A_\mu^d A_\nu^e
- \tilde{Z}_1 \partial_{\mu} \phi^a \partial_{\mu} \phi^a + \tilde{Z}_1 g f_{abc} \partial_{\mu} \phi^a \partial_{\mu} \phi^b A_\mu^c
$$

(1.17)

The $Z$s are the renormalization constants of the corresponding terms of the original Lagrangian. The explicit forms of the $Z$s can be found in [26]. Due
to the gauge invariance requirement, the coupling constants must be universal, which means that many of the $Z$s are related, e.g. $g_{0,Y,M} = \tilde{g}_0 = \frac{Z_{\Delta Y}}{Z_{\Delta Y,M}} = \frac{\tilde{Z}_1}{Z_1}$.

These relations are guaranteed by the Slavnov-Taylor identities [29] which are a consequence of the BRS (Becchi-Rouet-Stora) transformation [22].

The key point of the renormalization process is that no "new terms" are introduced: all the renormalized terms in $\mathcal{L}^{\text{vac}}_R (1.17)$ have the same structures as the corresponding terms in the original Lagrangian (1.10).

### 1.2.4 Renormalization Group Equation

According to the renormalization process, all divergences are subtracted from the Green's function systematically, order by order in perturbation theory. In the subtraction procedure there exists an arbitrariness of how to define a divergent piece in the Green's function. Summing up, the arbitrariness in subtracting divergences is two-fold:

1. arbitrariness of choosing the renormalization condition (i.e. setting up the condition to subtract divergences).

2. arbitrariness of fixing the renormalization scale $\mu$ (i.e. the mass scale at which the subtractions made).

Due to this arbitrariness, there exist many possible expressions for one physical quantity depending on the choice of the renormalization scheme. Since they are obtained from one physical quantity starting from the unique $\mathcal{L}$, and they describe a unique physical phenomenon, they thus have to be equivalent. The above statement is the idea of Renormalization Group (RG): the physical content of the theory should be invariant under the transformations that merely change the normalization conditions. An analytic expression of this property is given by the RG equation. The renormalization group equation expresses
the effect of a scale change in the theory or, more accurately, expresses the connection of the renormalizability to scale $\mu$ transformations. By the above definition, the RG equation must be a differential equation expressing the response of the Green's function and parameters (e.g. coupling constant and masses) to the change of renormalization scale $\mu$ [27, 30, 31].

For a $\mathcal{N}$ point Green's function with $\mathcal{N}_g$ gluons, $\mathcal{N}_c$ ghosts and $\mathcal{N}_v$ quarks, consider the relation between the bare $\Gamma_0$ and the renormalized vertex functions $\Gamma_R$:

$$
\Gamma_R(p_1 \cdots p_n, \alpha, \xi, m, \mu) = \lim_{\epsilon \to 0} Z_\Gamma \Gamma_0(p_1 \cdots p_n, \alpha_0, \xi_0, m_0, \epsilon)
$$

(1.18)

where $Z_\Gamma$ is the total renormalization constant $Z_\Gamma = (Z_{\Gamma_{W-A}}^{\frac{1}{2}})^{\mathcal{N}_g} (Z_{\Gamma_1}^{\frac{1}{2}})^{\mathcal{N}_c} (Z_{\Gamma_2}^{\frac{1}{2}})^{\mathcal{N}_v}$. $\alpha$ is the coupling constant, $\xi$ the gauge parameter, $\mu$ the renormalization mass scale. From (1.18), one finds that there is no $\mu$ dependence on the right-hand side term $\Gamma_0$. As mentioned before, the $\mu$ dependence is an artifact of the renormalization process, and can be compensated in the parameters $\alpha$ and $m$.

We introduce a dimensionless parameter $\chi = m/\mu$, and perform the $\mu \frac{d}{d\mu}$ operation on both sides of (1.18), the RG group equation can be obtained:

$$
\left( \mu \frac{\partial}{\partial \mu} + \beta(\alpha) \frac{\partial}{\partial \alpha} + \delta(\alpha) \frac{\partial}{\partial \xi} - \sum_i \gamma_i \chi_i \frac{\partial}{\partial \chi_i} - \nu \right) \cdot \Gamma_R = 0
$$

(1.19)
where the beta function $\beta(\alpha)$, anomalous mass dimension $\gamma_m$, the $\delta$ function and $\nu_T$ are defined as follows:

\[
\begin{align*}
\frac{d\alpha}{d\mu} &= \alpha \beta(\alpha) \\
\frac{\mu}{m} \frac{dm}{d\mu} &= -\gamma_m \\
\frac{\mu}{d\mu} \frac{d\xi}{d\mu} &= \xi \delta \\
\frac{\mu}{Z_T} \frac{dZ_T}{d\mu} &= \nu_T
\end{align*}
\]

(1.20)

The renormalization group equation represents the idea that one set of predictions with a renormalization scale choice $\mu = \mu_1$ can be related to another choice $\mu = \mu_2$ by the above two equations. Thus the RG equation (1.19) together with the $\beta, \gamma_m$ functions guarantee that our theory is based on a unique $\mathcal{L}$ and will give unique physical predictions independent of renormalization scale $\mu$.

### 1.2.5 Scaling and Asymptotic Freedom

What we mean by scaling is the response of the RG equation and the renormalization parameters such as the coupling constant and the mass $\nu_T$, when scaling all momenta by a factor $e^t$. The motivation of studying the scaling effect in quantum field theory was the experimental evidence of Bjorken scaling in deep inelastic scattering in $e - p$ collision [32]. The physical meaning of scaling momentum (i.e. the change with $t$) in a physical process is to change the dependence on the $\alpha, \xi, m$ to their running quantities. Any function in a field theory depends on a set of four-momentum ($p_i$), and on the parameters of the theory (such as the coupling constant and the mass), denoted generally by $g_i$. Replacing the $p_i$ by $\eta p_i$, one can ask how things depend on $\eta = e^t$ as $\eta$ increases from 1 to $\infty$. The renormalization group analysis allows the $\eta$
dependence to be shifted from the momentum variables to effective parameters
$g_i(\eta)$ which are scale $\eta$ dependent. These functions are defined as solutions to
certain differential equations (RG equations), which are further determined by
the structure of the theory [26].

Let us scale all momenta by a factor of $\eta$. $p_i = \eta p_i$. By dimensional analysis,
we find that the $N$ point Green’s function $\Gamma_R$ satisfies

$$
\Gamma_R(\eta p_1, \ldots, \eta p_N, \alpha, \xi, m, \mu) = \eta^{d_\Gamma} \Gamma_R(p_1, \ldots, p_N, \alpha, \xi, m, \mu/\eta)
$$

(1.21)

where $d_\Gamma$ is the mass dimension of the $N$ point Green’s function $\Gamma_R$. Together
with (1.19) and set $\eta = e^t$, one obtains the fundamental equation of the RG
involving the scaling parameter $t$.

$$
\left[ -\frac{\partial}{\partial t} + \beta(\alpha) \frac{\partial}{\partial \alpha} + \delta(\alpha) \frac{\partial}{\partial \xi} - \sum_i \gamma_i(\alpha) \frac{\partial}{\partial \lambda_i} - \nu - d_1 \right]
\cdot \Gamma_R(e^t p_1, \ldots, e^t p_N, \alpha, \xi, m, \mu) = 0
$$

(1.22)

The general solution of the above equation can be obtained via the method of
characteristics to solve linear partial differential equations. The general form
is as follows:

$$
\Gamma_R(\eta p_1, \ldots, \eta p_N; \alpha, \xi, m, \mu) = \eta^{d_\Gamma} \Gamma_R(p_1, \ldots, p_N; \tilde{\alpha}(t), \tilde{\xi}(t), \tilde{m}(t), \mu) \cdot e^{-\int_0^t \frac{dz}{\nu - d_1}}
$$

(1.23)

where the quantities $\tilde{\alpha}, \tilde{\xi}$ and $\tilde{m}$ are determined by the following first order

---

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ordinary differential equations:

\[ \frac{d}{dt} \tilde{a}(t) = \tilde{a}(t)[J(\tilde{a}(t))], \quad \tilde{a}(0) = \alpha \]  
\[ \frac{d}{dt} \tilde{\xi}(t) = \tilde{\xi}(t)[J(\tilde{a}(t))\cdot \tilde{\xi}(t)], \quad \tilde{\xi}(0) = \xi \]  
\[ \frac{d}{dt} \tilde{\chi}(t) = -\tilde{\chi}(t)[1 + \gamma_m(\tilde{a}(t), \tilde{\xi}(t)), \tilde{\chi}(t)], \quad \tilde{\chi}(0) = \chi \]

The beta function \( J(\alpha) \) (1.24) is of extreme importance because it determines the running coupling constant and hence further determines the strength of the interactions of the quantum field theory. The calculation of the beta function and the \( \gamma_m(\alpha) \) have been performed up to four loops order \( \mathcal{O} \).

In two-loop approximation the beta function is:

\[ J(\alpha) = \left( \frac{\alpha}{\pi} \right) J_1 + \left( \frac{\alpha}{\pi} \right)^2 J_2 + \mathcal{O} \left( \left( \frac{\alpha}{\pi} \right)^3 \right) \]

where \( \alpha \) is the running coupling constant related to \( g \) by \( \alpha = g^2/4\pi \). In SU(3) cases with three flavour degrees of freedom (i.e. 3 flavour and 3 colour freedom), \( J_1 = -9/2 \) and \( J_2 = -8 \).

With the help of the beta and the \( \gamma_m \) functions, it is not difficult to calculate the running coupling constant and the running mass. We choose the momentum scale to be \( \epsilon^4 = \sqrt{-q^2}/\mu \), where \( q \) is the typical momentum under consideration and \( \mu \) the fixed momentum scale (it is chosen to satisfy \( \tilde{a}(0) = \alpha \)).

Here we define a new momentum scale \( \Lambda \), where \( \Lambda \) is renormalization group invariant [26]:

\[ \ln(\Lambda^2) = \ln(\mu^2) + \pi/(\gamma_1 \alpha(\mu)) \]  

The momentum scale \( \Lambda \) is often referred as the QCD scale parameter and is one of the free parameters of QCD theory, which has to be fixed by experiments.
However, it is possible to set some a priori limit which $\Lambda$ is the value the running coupling becomes too large and perturbative theory breaks down. The typical value for $\Lambda = 300 \text{ MeV}$.

After inserting the two-loop beta function (1.27) into (1.24), we find the two-loop running coupling constant and the two-loop running mass provided $-q^2 \gg \Lambda$ [26]:

$$
\alpha(-q^2) = \alpha^{(2)}(q^2/\Lambda^2) \left\{ 1 - \alpha^{(2)}(q^2/\Lambda^2) J_1 \frac{\pi}{J_2} \frac{1}{2} \ln \left[ \frac{\pi (-q^2/\Lambda^2)}{\Lambda^2} \right] \right\}
$$

(1.29)

where $J_1$ and $J_2$ have the values given before, and $\alpha^{(2)}(q^2/\Lambda^2)$ is defined as:

$$
\alpha^{(2)}(q^2/\Lambda^2) = \frac{\pi}{-J_1 \frac{1}{2} \ln (-q^2/\Lambda^2)}
$$

(1.30)

$$
\hat{m}(-q^2) = \frac{\hat{m}}{\left( \frac{1}{2} \ln (-q^2/\Lambda^2) \right) \frac{\gamma_1}{J_1}} \left\{ 1 + \frac{\gamma_1 J_2}{J_1^2} \frac{1}{1/2 \ln (-q^2/\Lambda^2)} - \frac{\gamma_2 J_2 \ln \left( 1/2 \ln (-q^2/\Lambda^2) \right)}{J_1 \frac{1}{2} \ln (-q^2/\Lambda^2)} \right\}
$$

(1.31)

$\hat{m}$ is the RG invariant mass. $J_1$ and $J_2$ are defined before. $\gamma_1 = 2$ and $\gamma_2 = \frac{91}{12}$ in $SU_C(3)$ case.

In order to demonstrate the asymptotic freedom property in QCD and simplify our notation, let us just consider the one-loop case. In the one-loop situation, the beta function has the form of Eq.(1.27) with the $J_2$ set to zero. The important result is that the $\beta(\alpha)$ is negative for sufficiently small $\alpha$ as long as the number of quark flavour $N_f < 16$ (for the time being, we have experimental evidence for 6 quarks only). Note, in this case, both the $J_1$ and $J_2$ are negative, so the two-loop correction to the beta function (1.27) also contributes to its negativeness.
This unique feature of QCD (locally gauge invariant non-Abelian vector gluon theory) is entirely due to gluon self-interaction contributions. At one-loop level this is the triple-gluon vertex contribution to the two-point function $\Gamma_2$. From this one-loop beta function, the effective running coupling can be derived:

$$\alpha(t) = \frac{\alpha(0)}{1 - \frac{a}{\pi} \beta_0 t} \quad (1.32)$$

Because of the negativeness of $\beta_0$ in $N_f \leq 16$ cases, we find when $t \to \infty$ (ultraviolet limit), the running coupling constant $\alpha(t)$ approaches zero, i.e., the asymptotic freedom property: the larger the scale parameter (the larger the momentum), or the smaller the distance between particles, the smaller $\alpha(t)$ becomes and thus the more reliable the perturbative theory becomes for the strong interactions. This is the enormous advantage and the beauty of the QCD. Asymptotically the theory becomes a free field theory.

In summary, among the known renormalizable quantum field theories in four dimensions only QCD (Yang-Mills theory in general) enjoys the property of asymptotic freedom due to the gluon self-interactions. The experimental proof of QCD's asymptotic freedom comes from the deep inelastic scattering in which quarks behave like free particles ($\alpha \to 0$) at high energy ($t \to \infty$). Therefore, we are safe to use perturbation theory in the large momentum region of QCD, but in the low momentum region, the running coupling constant becomes large, and especially when the momentum decreases to the order of QCD scaling parameter $\Lambda$, the coupling constant becomes so large that the perturbation theory is no longer meaningful. In the low momentum region, there remain many unresolved problems which will be discussed in the next section.
1.3 Non-perturbative QCD

As we know, a lot of phenomena that can be studied in a field theory rely on perturbation theory. In QCD the miracle of asymptotic freedom, that is, the fact that the running coupling constant ($\alpha_s$) becomes small at short distances, allows us to use perturbative methods to study many interesting and important physical phenomena provided that we restrict ourselves to kinematic regions where the effective coupling constant becomes small enough. Nonetheless, the vast majority of events in a typical hadronic reaction fall into a kinematic region where perturbative QCD can not be employed ($\alpha_s$ too large). Examples include the fundamental issue of confinement, the determination of hadronic masses and decay widths, vertex functions, etc. It is thus of the utmost importance to find approaches to QCD calculations which extend a perturbative expansion in $\alpha_s$. Much has been achieved in the low-energy non-perturbative region of the QCD spectrum. Only two of the most active areas of this topic, QCD sum-rules and semi-classical instanton approach of QCD vacuum, will be presented. Other non-perturbative QCD approaches such as lattice gauge theories and effective-field theories are beyond the scope of this thesis.

1.3.1 Basis of QCD Sum Rules

A QCD sum-rule is an analytical method designed to provide an approximate calculation scheme for strong coupling QCD and in particular to account for non-perturbative effects [34]. The basis of the method are certain ideas of the structure of QCD vacuum and the knowledge of the short distance properties of QCD. Another equivalent definition is: the method of expansion of the correlation function in the vacuum condensates with the subsequent matching via the dispersion relation [35]. In this approach, we will encounter Wilson's operator product expansion (OPE) methods [36, 37] which take into account the
QCD vacuum condensate effects, and then in the spirit of duality, with the elegant Borelization technology, through the dispersion relation, QCD sum-rules have the power of predicting hadronic properties such as low-lying resonance masses, decay constants, etc.

First let us start from hadronic currents. The original Lagrangian (1.3) is built from the basic microscopic degrees of freedom of QCD, quarks and gluons. Neither quarks nor gluons are asymptotic states. Only hadrons that are colour-singlet bound states are experimentally observed. In order to study the properties of hadrons, it is convenient to start from empty space, the vacuum, inject there a quark and antiquark pair, and then follow the evolution of the valence quarks injected into the vacuum medium.

How to achieve the injection? The injection is achieved by external hadronic currents. The currents are built of quarks and gluons in such a way that the currents carry internal quantum numbers, such as charge or hypercharge, which coincide with the hadrons of interest. For example, the $I = 1$ case ($a_0$ meson) and the $I = 0$ case ($f_0$ meson) scalar currents are:

$$j_{I=0,1}(x) = [m_u \bar{u}(x) u(x) \pm m_d \bar{d}(x) d(x)]/\sqrt{2}$$ (1.33)

The most common currents are the vector and axial-vector currents since they actually exist in nature: virtual photons and W bosons couple to vector and axial-vector currents. Therefore, they are experimentally accessible in the reaction $e^+e^- \rightarrow hadrons$ or hadronic $\tau$ decays.

After constructing the hadronic currents, one needs to calculate the correlation function of the current. Basically, all QCD calculations start from the correlation function which is defined as:

$$\Pi(q^2) = i \int d^4x e^{iq \cdot x} \langle O| T(J(x)J(0))|O \rangle$$ (1.34)
Graphically, the correlation function $\Pi(q^2)$ is the amplitude for a quark and its own antiquark created by a source at point 0 to meet again at point $x$. Also it should be understood that the injected current carries a total four momentum of $q^2$.

The imaginary part of $\Pi(q^2)$ for $q^2 > 0$ (i.e., above the physical threshold of hadron production) is called the spectral density $\rho(s)$. ($\rho(s) = 4\pi Im \Pi(s)$. $\sim \equiv q^2$). Up to normalization, it coincides for vector currents with the cross section of $e^+e^- \rightarrow \text{hadrons}$ and the axial-vector for the $\tau$ decay distribution function. so the spectral density $\rho(s)$ carries full information about the spectrum of hadrons with given quantum numbers. Calculating the spectral density exactly in a systematic way is every theoretical physicist's dream, and because of the difficulties in the non-perturbative QCD regime, at present only approximate methods can be used in practical calculations.

Having obtained the spectral density, the total hadronic decay rate of the given current can be written as $R = \int_0^{M^2} ds \rho(s)$. but since the hadron spectral functions are sensitive to the non-perturbative effects of QCD, the integrand can't be directly calculated at present in any systematic way. Nevertheless, the integral itself can be calculated systematically by exploiting the analytic properties of the correlation functions $\Pi(s)$ [38]. The correlators are analytic functions of $s$ except along the positive real $s$ axis where their imaginary parts have discontinuities. So the integral of $\rho(s)$ can therefore be expressed as a contour integral running from $s = M^2 - i\epsilon$ below the axis to $s = M^2 + i\epsilon$ above the axis. Referring to Figure 1.3, the integral could also have singularities at $Q^2 = 0$. By analyticity, the integral around the closed contour vanishes. Thus $R$ can be expressed as an integral around the contour that runs counterclockwise around the circle $|s| = M^2$. The advantage of this expression of $R$ is that it requires the correlator only for complex $s$ of order $M^2$ which can be
significantly larger than the scale associated with non-perturbative effects of QCD.

One thing to mention here is that although our desired target is the spectral density \( \rho(s) \) on the physical cut (i.e. the positive value of \( q^2 \)), all theoretical calculations in QCD are carried out off the physical cut \( (Q^2 = -q^2 > 0) \). The reason is obvious: the QCD Lagrangian (1.3) is formulated in terms of quarks and gluons, not hadrons. So working in the Euclidean domain, off the physical cuts, one can calculate in terms of quarks and gluons, and dispersion relations are used to relate the Euclidean domain to the physical cuts.

To calculate the correlator in terms of quarks and gluons, one must use the Wilson OPE methods which are formulated in the Euclidean domain [36]. Wilson OPE is the basis of virtually all analytical calculations of non-perturbative effects in QCD, and is the theoretical basis of QCD sum rules. The central idea is that the time-ordered product of two local (elementary or composite) operators at short distances can be expanded in terms of a complete set of regular local operators \( \hat{O}_n(0) \) [36, 37].

\[
T[A(x)B(0)] \approx \sum_n C_n^{AB}(x)\hat{O}_n(0) 
\]

The c-number coefficients \( C_n^{AB} \) are called Wilson coefficients.

The operators \( \hat{O}_n \) appearing in (1.35) are constrained by the symmetry properties of \( A(x), B(0) \) and the underlying quantum field theory. In the above equation, all short distance singularities are forced out from the local operator, and built into the c-number coefficients. Since the OPE studies short distance properties \( (x \to 0) \), the coefficients \( C_n^{AB}(x) \) can be determined perturbatively, independent of the process involved [39]. Thus in the OPE, we can separate short-distance and long-distance effects systematically, all the short-
Figure 1.3: Contour integral of the spectral density $\rho(s)$ in the complex $s$ plane where $\sigma = M^2$. $\rho(s)$ exhibits a discontinuity along the real $s$ axis.
distance perturbative effects are built into the singular c-number coefficient \( C_n \) and long-distance, non-perturbative effects are embedded in the regular local operator \( \hat{O}_n \). The separation of short-distance and long-distance effects is one of the advantages of the OPE method and enables the OPE to provide a useful extension of QCD into the non-perturbative regime. Usually the \( \hat{O}_n \) terms in (1.35) are organized in increasing mass dimension order, generally decreasing in importance as the dimension increases. In other words, because the total mass-dimension of \( A(x)B(0) \) is fixed, the coefficients \( C_n(x) \) are ordered according to decreasing order of singularity when \( x \to 0 \). Suppose operators \( A(x) \) and \( B(x) \) respectively have mass dimensions \( d(A) \) and \( d(B) \), and operator \( \hat{O}_n \) has mass dimension \( d(\hat{O}) \). For simplicity, all possible anomalous dimensions are omitted for now. we find

\[
C_n(x) \xrightarrow{\varepsilon \to 0} x^{\lambda_n}, \quad \lambda_n = -d(A) - d(B) + d(\hat{O}_n)
\]  

(1.36)

Fourier-transformation of (1.35) results in the following expression.

\[
\int e^{iq \cdot x} \langle \{T[A(x)B(0)]\}\rangle_d x = \sum_n \hat{C}_n(q^2) \hat{O}_n
\]  

(1.37)

where \( \hat{C}_n \) are regular c-numbers obtained from \( C_n \) in (1.35). By power counting, we find

\[
\hat{C}_n(q^2) \sim \frac{const}{(q^2)^{\frac{\lambda_n}{2}}}
\]  

(1.38)

the singularities are represented by the \( \frac{1}{(q^2)^{\frac{\lambda_n}{2}}} \) terms in the above equation.

The higher the dimension of local operators \( \hat{O}_n \), the less singular the coefficient \( C_n(x) \). Hence the dominant operators at short distance are those with the small mass dimensions. Because the OPE is formulated at short-distances.
the Fourier-transforming momentum $q^2$ is reasonably large, we can conclude that the higher the local operator's mass dimension, the less important its contribution to the OPE because of the suppression of $\frac{1}{(q^2)^{D-2}}$, and after Borel transformation the higher dimension operator's contribution will be further suppressed. Therefore another advantage of the OPE method is that it usually just involves a rather small number of operators. In practice, the operators which are used in OPE for parameterizing the non-perturbative effects are limited: $qq~;~GG~;~GGG~;~\bar{q}qGq~;~and~;~\bar{q}q\Gamma qq\Gamma q$. Definitions of these operators will be discussed later.

1.3.2 Vacuum Expectation Values

In momentum space, applying the OPE to the two-point correlation function $\Pi(x)$, we have

$$\Pi(Q^2) = \sum_n C_n(Q^2) \langle \hat{O}_n \rangle_{vac}$$

where the $C_n(Q^2)$ are the c-number functions as usual. and the $\langle \hat{O}_n \rangle_{vac} = \langle \Omega | \hat{O}_n | \Omega \rangle$ are vacuum expectation values (VEV) of QCD operators, collectively known as the condensates. The $\langle \Omega \rangle$ is the true QCD vacuum.

The above operator-product expansion (1.39) must respect the symmetries of the quantum field theory being considered, placing restrictions upon the VEV appearing in the OPE. For a gauge invariant current in QCD, the VEV $\langle \hat{O}_n \rangle$ must be gauge invariant [39, 40]. Applying OPE methods to a gauge invariant, scalar correlation function $\Pi(Q^2)$ in momentum space [41, 42, 43].

$$\Pi^{QCD}(Q^2) = \Pi^{pert}(Q^2) + \frac{a}{Q^2} \langle \alpha GG \rangle + \frac{b}{Q^4} \langle m \bar{q}q \rangle + \frac{c \cdot m_q^2}{Q^4} \langle \bar{q}G \cdot \sigma q \rangle$$

$$+ \frac{d \cdot m_q^2}{Q^6} \langle \alpha GGG \rangle + \frac{e}{Q^4} \langle \alpha (\bar{q}q)^2 \rangle$$

(1.40)
where $m_q$ is the light quark mass in the $SU(2)$-flavour limit, which in the OPE domain is relatively small compared with momentum involved ($Q^2 \gg m_q^2$). The quantity $\Pi^{pert}$. coefficients $a, b, c, d$ and $e$ can be calculated from perturbative calculations.

The coefficients can be calculated by perturbative methods but the values of the VEV condensates cannot be obtained from first principles. There are two sources for the determination of the VEV condensates. First, one may study many different physical current correlation functions which all involve the same basic set of unknown VEVs. Second, some of the VEVs are already estimated phenomenologically from current algebra studies, such as the Partially Conserved Axial-vector Current (PCAC).

The lowest dimension (zero) belongs to the trivial unit operator. When one calculates the perturbative contribution to the correlator $\Pi(Q^2)$, one actually calculates the coefficient of the unit operator.

The operator of the next lowest dimension (three) is the quark density operator $O_q = \bar{q}q$. In the chiral limit (i.e., when the quark mass term in the Lagrangian (1.3) is set to zero) $O_q$ is the order parameter whose VEV signals the spontaneous breaking of the axial $SU(N_f)$ symmetry and the occurrence of the corresponding massless pions via the Goldstone mode [44]. In perturbation theory, the chiral symmetry remains unbroken and $\langle O_q \rangle$ vanishes identically. It is tempting to say that $\langle O_q \rangle \neq 0$ measures the derivations from the perturbation theory. The value $\langle \bar{m}qq \rangle$ is determined from the theory of chiral symmetry breaking according to Gell-Mann-Oakes-Renner and using the PCAC relation described in [34, 45]. A more detailed discussion will be presented later in this thesis. PCAC gives $(m_u + m_d)(\bar{u}u + \bar{d}d) = -m_\pi^2 f_\pi^2$, where $f_\pi$ is the pion constant and $m_\pi$ is the pion mass.

The next highest dimension operator is the gluon condensate $\langle O_{\gamma \gamma} \rangle$. The
gluon-condensate is closely related to the semiclassical QCD vacuum structure
instanton effects, and we will discuss this in more detail later in the thesis.

The dimension-five operator is the mixed quark-gluon operator
\( \langle O_{qG} \rangle = \langle \bar{q} \sigma G q \rangle \). From (1.40), we know that this operator’s contribution to
the scalar channel’s OPE is proportional to \( \frac{m_q}{Q^2} \), so in the light quark case with
relatively large momentum transfer, this operator plays a negligible role in the
\( I = 1.0 \) channel sum rules. It is very important, however, in a wide range of
problems involving baryons [46], and mesons built from one light quark and
one heavy quark [47].

At the level of dimension six, there is one operator built from three gluon
field tensors \( \langle \alpha, fGGG \rangle \) and several four-quark operators of the type
\( O_{q4} = \langle \bar{q}_1 \Gamma_1 q_2 \rangle \langle \bar{q}_3 \Gamma_2 q_4 \rangle \) where \( \Gamma_{1,2} \) denote certain flavour-conserving combina-
tions of the Lorentz and colour matrices and \( q_i \) is the light quark field of
different flavours (e.g. u, d, s). The three-gluon operator is expected to have a
significant impact in heavy quarkonium [48]. It is determined from the Instan-
ton vacuum calculation [49] and it does not appear in the lowest order \( I = 0.1 \)
meson sum rules because the three-gluon operator’s effect is also proportional
to \( \frac{m_q}{Q^2} \) as shown in (1.40).

As for the four-quark operators, their VEVs are not known independently.
The standard way to evaluate them is a vacuum saturation approximation,
which means the four-quark operator can be represented by the product of two
two-quark operators [34]. i.e.

\[
\langle O_{q4} \rangle = \langle \bar{q}_1 \Gamma_1 q_2 \rangle \langle \bar{q}_3 \Gamma_2 q_4 \rangle + \text{permutations} \quad (1.41)
\]
1.3.3 Spontaneous Symmetry Breaking

For the sake of brevity, the Lagrangian is defined as follows without gauge-fixing and ghost terms.

\[
\mathcal{L} = -\frac{1}{4} F^a_{\mu\nu} F^{a,\mu\nu} + \sum_f \bar{q}_f (i\gamma^\mu D_\mu - m_f) q_f
\]  

(1.42)

The QCD Lagrangian with \( N_f \) massless flavours \( m_f = 0 \) is known to possess a large global symmetry, namely a symmetry under \( SU(N_f)_L \otimes SU(N_f)_R \) independent rotations of left- and right-handed quark fields. This symmetry is called chiral symmetry. After setting \( m_f = 0 \) in the above equation, the QCD Lagrangian splits into two independent quark sectors:

\[
\mathcal{L} = -\frac{1}{4} F^a_{\mu\nu} F^{a,\mu\nu} + i \bar{q}_L \gamma^\mu D_\mu q_L + i \bar{q}_R \gamma^\mu D_\mu q_R
\]  

(1.43)

Here \( q \) denotes the flavour vector \( q = (u, d, s, \cdots) \), and \( q_L, q_R \) stand for left and right handed components of the quarks. \( q_L = (\begin{pmatrix} 1 \\ i \\ 0 \\ 0 \end{pmatrix})q \), \( q_R = (\begin{pmatrix} 0 \\ 0 \\ 1 \\ i \end{pmatrix})q \). The definition of \( \gamma_5 \) can be found in Appendix I. From the above definitions, we find the two quark chiralities live in separate flavour space which do not talk to each other (gluon interactions do not change the chirality).

Instead of rotating the left- and right-handed quark fields separately, one can make equivalent independent vector and axial vector \( U(N_f) \) rotations of the full 4-component Dirac spinors, which means that the QCD Lagrangian is invariant under these transformation too in the massless quark cases. In the case of \( m_u = m_d = 0 \), a vector rotation is denoted as \( \psi(x) \rightarrow e^{-i \alpha_a(x) \gamma^a} \psi(x) \). and an axial rotation is \( \psi(x) \rightarrow e^{-i \alpha_a(x) \gamma^a \gamma_5} \psi(x) \). Under these transformations, the QCD Lagrangian remains invariant.

The reason why \( \bar{\psi}(x) \gamma_\mu \psi(x) \) is invariant is that \( \gamma_5 \) anticommutes with every
\( \gamma \) matrix. Thus any bilinear form with an even number of \( \gamma \) matrices between \( \psi^T(x) \) and \( \psi(x) \) is chirally symmetric, and all bilinear terms with an odd number are not. Consequently the quark-mass term \( m_\bar{q}q \) in Eq. (1.42) violates the symmetries, but since the current-mass of \( u \) and \( d \) quarks are small (\( m_u \approx 4 \MeV \), \( m_d \approx 7 \MeV \)), their symmetry breaking effects should be weak.

If the axial rotation is a chiral symmetry operation, the chiral partner \( \rho \) and \( a_1 \) should have the same mass. In reality, the split between the chiral partners \( \rho \) and \( a_1 \) is very large \( m_{a_1} - m_{\rho} \approx 1260 - 770 \approx 500 \MeV \) \cite{50}. This phenomenon implies that in addition to the small explicit breaking of chiral symmetry, there must be spontaneous symmetry breaking (SSB). SSB means a symmetry present in the Lagrangian is not presented in the actual physical ground states. Equivalently, the vacuum itself breaks the symmetry.

If axial transformations are a symmetry operation, it should follow that \( Q_5^a = \int d^4x \bar{\psi}(x) \gamma_0 \gamma_5 \tau^a \psi(x) \) is an additional conserved quantity, similar to the total isospin \( Q^a = \int d^4x \bar{\psi}(x) \gamma_0 \tau^a \psi(x) \). According to Noether's theorem, the axial current \( J_5^a = \bar{\psi}(x) \gamma_5 \tau^a \psi(x) \) should also be conserved (i.e. \( \partial_\mu J_5^\mu = 0 \)). On the other hand, we just argued that this symmetry is spontaneously broken for the ground state; thus \( \hat{Q}_5|O\rangle \neq |c_1\rangle \neq 0 \). To lowest order, we find \( \langle O|J_5^\mu|c_1\rangle \neq 0 \). The \( |c_1\rangle \) should be identified with some field which could be related to any pseudoscalar. In the absence of chiral symmetry breaking, since \([\hat{H}_0, \hat{Q}_5] = 0\), it follows that \( \hat{H}_0|c_1\rangle = \hat{Q}_5 \hat{H}_0|O\rangle = 0 \), which means the particle must be massless (it is the corresponding, so-called Goldstone boson). The pion with its extremely small mass is the natural candidate for the Goldstone boson. Immediately following the above relation comes the famous PCAC relation:

\[
\partial_\mu J_5^\mu = f_\pi m_\pi^2 \pi(x) \tag{1.44}
\]

38
This equation implies that the violation of axial-vector current conservation can be described as being due to the coupling to pions. From this starting point, one can obtain the famous quark condensate relationship:

\((m_u + m_d)(O|\bar{u}u + \bar{d}d|O) = -f_\pi^2 m_\pi^2\), where \(f_\pi = 93 \text{ MeV}\) and \(m_\pi = 140 \text{ MeV}\).

It has been seen that the non-perturbative effects lead to the introduction of a quark condensate. In perturbative QCD, the axial symmetry remains unbroken and \(\langle \bar{q}q \rangle = i \int d^4x \text{Tr}[S(x,x)]\) which vanishes identically.

In the SU(3) limits \((m_u = m_d = m_s = 0)\), the QCD vacuum breaks the axial symmetry accordingly (after the symmetry breaking of the remaining \(U(3)_L \otimes U(3)_R\) symmetry, the axial SU(3) and the U(1) symmetry are not manifest in the particle degeneracies). The Goldstone theorem then informs us that there should be \(N_f^2 - 1 = 8\) approximately massless Goldstone mesons in the hadron spectrum for the breaking of axial SU(3) symmetry [45, 51]. The eight Goldstone bosons can be identified readily as the three pions, four kaons and one \(\eta\) meson. However, since we need to break an extra axial U(1) symmetry, we are still one pseudoscalar short. The natural candidate is the remaining pseudoscalar is \(\eta'\), but its mass is far too large \((m_{\eta'} \sim 960 \text{ MeV})\) [50] to be identified as a Goldstone boson. This is the famous U(1) problem.

Anomalies in perturbation theory were first observed in 1969 [52, 53]. Anomaly means the loop diagram involving external vector and axial-vector currents could not be regulated in such a way that all the currents remained conserved and the axial current becomes nonconserved. From the triangle diagram involving two gauge fields and the flavour singlet axial current, one finds [45]:

\[
\partial_\mu j_\mu^5 = \frac{N_f}{16\pi^2} F_{\mu\nu}^a \tilde{F}_{\mu\nu}^a \tag{1.45}
\]
This result is not modified at higher order corrections in perturbation theory. The fact that the flavour singlet current has an anomalous divergence was welcome in QCD because it can be used to explain the absence of a ninth Goldstone boson. The right-hand side of the above equation is related to the famous instanton solution which will be discussed later. The fact that the PCAC-type consideration cannot be applied to the \( \eta' \) implies its mixture with the gluonic world through the operator \( \tilde{F}F \).

In summary, SSB refers to the breaking of \( SU(N_f)_L \otimes SU(N_f)_R \) chiral symmetry for the QCD of \( N_f \) massless quarks into the \( SU(N_f)_V \) symmetry, which must have \( N_f^2 \) almost massless Goldstone bosons according to Goldstone theorem. SSB seems to solve the hadron mass degeneracy problems and the \( U(1) \) puzzle successfully, both of them connected deeply with the non-perturbative effects of QCD. The quark condensate is the order parameter of chiral symmetry and the \( \eta' \) problem is related to \( \tilde{F}F \).

### 1.3.4 Dispersion Relations and Duality

Using several phenomenological numbers (\( \Lambda, \langle mqq \rangle, \langle GG \rangle \)) and the quark masses as input, QCD practitioners are able to employ the OPE method with the help of dispersion relations to understand an enormous wealth of the data referring to low-energy hadronic physics. In the ideal world, one would calculate the correlator \( \Pi(Q^2) \) and the spectral density proportional to \( \text{Im}\Pi(s) \) exactly. In reality one has to calculate \( \Pi(Q^2) \) in the OPE method in the form of a truncated series. This calculation is done in the Euclidean domain (positive \( Q^2 \)) and in terms of quarks and gluons. The complication comes from the fact that all physical observables (such as cross section, decay width, mass etc.) are measured in the Minkowski domain (\( q^2 = -Q^2 > 0 \)). The connection between the Euclidean predictions and the measurable quantities is established
via dispersion relations.

Kallen and Lehmann quite long ago showed that two-point function obeys a dispersion relation [54. 55]. The dispersion relation follows from the analytical properties of \( \Pi(Q^2) \) as a function of \( Q^2 \). The only energy-momentum invariant which appears in a two-point function. The dispersion relation is:

\[
\Pi(Q^2) = \int_0^\infty dt \frac{1}{t + \frac{Q^2}{\pi}} \text{Im} \Pi(t) + a + bQ^2 + \cdots
\]  

where the degree of polynomial in the right-hand side depends on the convergence properties of \( \text{Im}(t) \) when \( t \to \infty \). The analyticity of \( \Pi(Q^2) \) apart from a branch cut along the negative real axis \( (Q^2 < 0) \) is used to prove this dispersion relation [56]. As we mentioned before, the interest of this representation is the spectral function \( \frac{1}{2} \text{Im} \Pi(t) \). With \( J(x) \) a current with specific quantum numbers, the spectral function is then directly related to the total cross-section for the production of the hadronic states with these quantum numbers.

In summary, we have the widely used dispersion relation equation \( (Q^2 = -q^2) \):

\[
\Pi(Q^2) = \frac{1}{\pi} \int_0^\infty \frac{ds}{s + Q^2} \frac{\text{Im} \Pi(s)}{s} + \text{const.}
\]  

The key element of every calculation referring to Minkowskian quantities is quark-hadron duality where a truncated OPE is analytically continued term by term from the Euclidean to the Minkowski domain [57. 58]. The smooth quark curve obtained in this way is supposed to coincide at high energies with the actual hadronic cross-section. If duality is formulated in this way, it is obvious that at finite energies deviations from duality must exist because of the differences between the measured physical cross-section and a smooth OPE prediction. The deviation from duality is due to the omitted components in the
OPE calculation and it will arise when one try to predict the spectral density \( Im\Pi(s) \) point-to-point at large \( s \).

The OPE-based predictions require additionally a different type of duality. One needs to assume that a particular cut of interest in the hadronic amplitude is in one-to-one correspondence with the given quark-gluon cut. In other words, it is assumed that different channels (in terms of hadronic process and in terms if quark-gluon process) do not contaminate each other [59]. This is the so-called "global duality" [60]. In the OPE calculations, the cut of the perturbative coefficient functions carries has identity, and the above global duality is easily implemented. In this thesis, the global duality is assumed always valid, and the duality in this context simply means the local duality.

It has been shown that the difference between the exact result and the series truncated at optimal order in the OPE is exponential [61, 62]. Instantons, treated in an appropriate way will represent the omitted terms in the truncated series [63]. The instanton contribution to the correlation function with large momentum transfer can be graphically interpreted as a mechanism in which the large external momentum is transmitted through a soft coherent field configuration. i.e. the large external momentum is shared by a very large number of quanta so that each quantum is still relatively soft. It is clear that this mechanism is not represented in the OPE, and thus gives an idea of how strong deviations from duality might be. The exponential terms not seen in the OPE appear both in the Euclidean and Minkowski quantities. The rate of fall off is much faster in the Euclidean domain than in the Minkowski domain. Conceptually, the exponential terms in the Minkowski domain determine the deviations from duality. Because the exponential deviation from duality can be related to the existence of instantons, we will leave this topic for the instanton part of this thesis.
1.3.5 Borel Transformation and Sum Rules

In practical applications of the sum-rule method there is a technical method needed in addition to dispersion relations in order to study the low-energy aspects of QCD. The method referred to is Borelization (comes from the Borel transformation) [26, 34], and it consists in applying the following operator $\hat{B}$ to the function under consideration:

$$\hat{B} = \lim_{Q^2 \to -\infty} \frac{(-Q^2)^n}{(n-1)!} \left( \frac{\partial}{\partial Q^2} \right)^n$$

(1.48)

with $M^2 = \frac{Q^2}{n} = \text{fixed}$. Applying the Borel transformation to the sum rule in (1.47), we have:

$$\Pi(M^2) \equiv \hat{B} \Pi(Q^2) = \frac{1}{\pi M^2} \int_0^\infty ds \, \text{Im} \Pi(s) e^{-s/M^2}$$

(1.49)

where the following relations have been employed [26]:

$$\hat{B} \left( \frac{1}{Q^2} \right)^n = \frac{1}{(n-1)!} \left( \frac{1}{M^2} \right)^n \cdot \hat{B} \left( \frac{1}{s + Q^2} \right) = \frac{1}{M^2} e^{-s/M^2}$$

(1.50)

The advantages in dealing with the Borel-transformed sum rules are obvious:

1. First, one improves factorially the convergence of the power series (1.50).
   This improved accuracy makes the prediction of lowest-lying resonance's properties more reliable.

2. On the phenomenological side, proceeding to the Borel-transformed dispersion relations we automatically kill all possible subtraction constants. Even more important, the exponential weight function in (1.49) makes the integral over the imaginary part well convergent. This weight func-
tion enhances the lowest-lying resonance's contribution in the integral while contributions of the higher-order resonances are exponentially suppressed.

It is worth mentioning that there are a wide variety of QCD sum rules that can be utilized [64]. They include the Laplace sum rules, the Finite Energy sum rules [64], the Gaussian Transform sum rules [56] and so on. Laplace sum rules have been most successful in applications.

Laplace sum rules employ the Borel transformation of the standard dispersion relation (such as Equation 1.49). The interesting point about this type of sum rules is the presence of the exponential factor in the integrand which gives a predominant weight to the low-energy component of the hadronic spectral function, thus the Laplace Sum-Rule is particular suitable for the determination of the properties of the lowest-lying resonances of mesons or baryons.

The simplest spectral model is a delta function plus continuum.

\[
\rho(s) = c_1 \delta(s - M^2) + \theta(s - s_0) Im \Pi^{QCD}(s)
\]

where the delta function represents the lowest-lying resonance contribution and the theta function represents the continuum contribution. This is the famous Shifman-Vainshtein-Zakharov (SVZ) QCD sum-rule spectral model [34].

There are some kinds of modified Laplace SR often used in the literature which are represented as \( R_k \) [64]. The quantity \( R_k \) is defined as:

\[
R_k(M^2, s_0) = M^2 \hat{B}[(q^2)^k \{ \Pi(Q^2) - \Pi(0) \}] - \frac{1}{\pi} \int_{s_0}^{-\infty} s^k e^{-s/M^2} Im \Pi(s) ds = \frac{1}{\pi} \int_{0}^{s_0} s^k e^{-s/M^2} Im \Pi^{QCD}(s) ds
\]
where $M^2$ is the Borel transformation parameter as we defined before and $s_0$ is the starting point of the continuum threshold. It is known that different ranks of $R_k$ have different suppression of the non-perturbative contribution and the lowest-lying resonance contribution. The higher rank $R_k$ enhance the continuum contribution and suppress the lowest-lying resonance’s contribution to the sum rules. The most used sum rules are $R_0$, $R_1$ \cite{65}.

In summary, QCD sum-rules begin with study of a correlation functions, graphically understood as an external current injected into the vacuum with very large momentum $Q^2$, in the deep Euclidean domain. The points of injection and annihilation of the quark pair in the vacuum are separated by a small space time interval, the injected quark hence has no time to interact with the vacuum medium. They propagate as free objects, and thus we get the perturbative part of QCD. For the non-perturbative part of QCD, the external current’s total energy is not large enough, the quark or antiquark, being injected, starts evolving according to the dynamical laws of QCD instead of acting as free particles. At first, the quarks do not feel the impact of the vacuum medium. As the separation between them grows, the effects of the medium became more and more important, eventually preventing quarks from appearing in the detectors (no free quarks). The injected quarks get dressed and materialize themselves in the form of hadrons \cite{35}.

The general steps for a QCD sum-rule calculation are:

1. Identify an appropriate interpolating field for the hadron of interest and construct a correlator function.

2. Identify the tensor structure and invariant functions of the correlator.

3. Write dispersion relations for each invariant function with a spectral model,
4. Construct the OPE for each invariant function,

5. Convert to Borel weighting,

6. Match and extract parameters of the spectral model.

1.3.6 Instantons

QCD sum rules are very successful in predicting some low-energy hadronic properties with just a few parameters as input, especially in the vector and axial-vector channels. But still there remain several contradictions which QCD sum rules could not answer.

QCD sum rules give very accurate prediction on vector and axial-vector channels, but provide incomplete results on spin-zero channels, both for current made of quark and gluon fields such as $\pi, \eta', \sigma$ and scalar glueballs. This problem is first emphasized by Novikov et al in 1981 [66]. For example, using QCD sum rules, we find to any order, the $a_0$ and $f_0$ meson's correlation functions are identical, which implies $a_0$ and $f_0$ should have the same masses. From the PDG data book we know there are several isospin-partner candidates for $a_0$ and $f_0$ with different masses [50]. This phenomenon indicates that something is missing and better control over high order corrections by OPE methods would not solve this puzzle.

The second problem is the famous $U(1)$ puzzle [51, 52]. Why is the $\eta'$ meson extremely heavy? It was in principle solved when it was realized that the $U(1)$ chiral symmetry was explicitly broken by the axial anomaly (see Section 1.3.3). However, the quantitative description of the $\eta'$ mass is still missing. It is noted that this second problem is deeply related to the problems of the spin-zero mesons.

QCD sum rules use the values of condensates as a first principle (the values
are determined from the experimental data rather than deriving them. A field theory method such as QCD which could not explain the origin of the condensates is an incomplete theory. The third question is this: Where do the condensates come from. or what is the quantitative picture of the QCD vacuum structure?

The concepts of instantons are a natural solution to the above three puzzles [63]. We will show how instantons solve these three puzzles step by step. First a pedagogical description of the instanton solution is given.

In addition to the global minimum of the QCD action $A^a_\mu = 0$ used by perturbation theory, there are many other local minima called instantons which have to be taken into account. Instantons are certain configurations of the Yang-Mills potentials $A^a_\mu (x)$ satisfying the equation of motion $D^{ab}_\mu A^b_\mu = 0$ in Euclidean space [67]. The solution has been found by Belavin, Polyakov et al in 1975 [68, 69]; the name “instanton” comes from the suggestion of ’t Hooft in 1976 [70], who made a major contribution to the investigation of instanton properties.

Physically, one can think of instanton in two ways. on one hand it is a tunneling process occurring in imaginary time (this interpretation belongs to V. Gribov) [71]), on the other hand, it is a localized pseudoparticle in the Euclidean space [69].

Before we study the tunneling phenomena in Yang-Mills theory, let us clarify the definition of the vacuum of the theory. In the Hamilton formulation, it is convenient to use the so-called Weyl gauge $A_0 = 0$ (here the notation $A_i = A^a_i \lambda^a / 2$, where the $\lambda^a$ is the normalized $SU(N)$ generator). In the Weyl gauge case, the conjugate momentum to the field variables $A_i(x)$ is just the
electric field $E_i = \partial_0 A_i$. The Hamiltonian is given by

$$H = \frac{1}{2g^2} \int d^4x (E_i^2 + B_i^2)$$ \hspace{1cm} (1.53)

where $E_i^2$ is the kinetic and $B_i^2$ the potential energy terms. The $B_i^a$ is defined as:

$$B_i^a(\vec{x}, t) = \frac{1}{2} \epsilon_{ijk} [\partial_j A_k^a - \partial_k A_j^a + \epsilon^{abc} A_j^b A_k^c]$$ \hspace{1cm} (1.54)

In the non-Abelian gauge theory, the classical vacuum corresponds to the gauge fields which have zero potential energy. One finds that if the field happens to be a pure gauge $A_i = i U \partial_i U^*$ (where the $U = U(\vec{x})$ is the gauge transformations), the potential energy at such points is naturally zero. Thus we define the classical vacua as $A_i = i U \partial_i U^*$.

In order to enumerate the classical vacua, we have to classify all possible gauge transformations $U(x)$. This means that we have to study equivalence classes of mapping from 3-space $\mathbb{R}^3$ into the gauge group $SU(N)$. In practice, we can restrict ourselves to matrices satisfying $U(\vec{x}) \to 1$ as $x \to \infty$ \cite{72}. Such mapping can be classified using an integer called the Pontryagin (or Winding) number, which counts how many times the group manifold is covered.

$$n_W = \frac{1}{24\pi^2} \int d^3x \epsilon^{ijk} Tr \left[ (U^* \partial_i U) (U^* \partial_j U) (U^* \partial_k U) \right]$$ \hspace{1cm} (1.55)

We conclude that there is an infinite set of classical vacua enumerated by an integer $n_W$. Since they are topologically different, one cannot go from one vacuum to another by means of a continuous gauge transformation. Therefore there is no path from one vacuum to another such that the energy remains zero all the way. The connection of different classical vacua has to be through
a tunneling effect. From the above quantum-mechanical example (1.53), we know that we have to look for classical solutions of the Euclidean equation of motion (the instanton). The best tunneling path is the solution with minimal Euclidean action connecting vacua with different winding number (the winding number in terms of corresponding gauge field $A_i$ instead of gauge transformation $U(x)$ is called the Chern-Simons number $n_{CS}$).

In order to minimize the action, we exploit the identity:

$$S = \frac{1}{4g^2} \int d^4x F^{a}_{\mu\nu} F^{a}_{\mu\nu}$$

$$= \frac{1}{4g^2} \int d^4x \left( \pm F^{a}_{\mu\nu} \tilde{F}^{a}_{\mu\nu} + \frac{1}{2} (F^{a}_{\mu\nu} \mp \tilde{F}^{a}_{\mu\nu})^2 \right)$$

(1.56)

where $\tilde{F}_{\mu\nu} = \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} F_{\rho\sigma}$ is the dual strength tensor. Since the first term in (1.56) is topological invariant which is determined by the topological charge (or four-dimensional Pontryagin index):

$$Q_T = \frac{1}{32\pi^2} \int d^4xF^{a}_{\mu\nu} \tilde{F}^{a}_{\mu\nu}$$

(1.57)

and the last term is always positive, it is clear that the action is minimal if the field is (anti) self-dual

$$F^{a}_{\mu\nu} = \mp \tilde{F}^{a}_{\mu\nu}$$

(1.58)

The above equation also can be used as the definition of the instanton because one can show directly that the self-duality condition implies the equation of motion $D_\mu F_{\mu\nu} = 0$ [63]. In addition to that, one can show that the energy-momentum tensor vanishes for the self-dual fields. In particular, the self-dual fields have zero (Minkowski) energy density. Insert the topological charge $Q_T$
(1.57) into the action (1.56). We find:
\[ S \geq \frac{8\pi^2}{g^2} |Q_T| \geq \frac{8\pi^2}{g^2} \]  \hspace{1cm} (1.59)

For finite-action field configuration, \( Q_T \) has to be an integer. This can be seen from the fact that the integrand is a total derivative.

\[
Q_T = \int d^4x \partial_\mu K_\mu = \int d\sigma_\mu K_\mu \]  \hspace{1cm} (1.60)

\[
K_\mu = \frac{1}{16\pi^2} \epsilon_{\mu\nu\lambda\sigma} \left( A_\alpha^a \partial_\beta A_\gamma^b + \frac{1}{3} f^{abc} A_\alpha^a A_\beta^b A_\gamma^c \right) \]  \hspace{1cm} (1.61)

Inserting the pure gauge \( A_\mu = iU \partial_\mu U^\dagger \) into the above equations, we find that \( Q_T = n \). Furthermore, if the gauge potential falls off rapidly at the spatial infinity.

\[
Q_T = \int dt \frac{d}{dt} \int d^3x K_0 = n_{CS|t=\infty} - n_{CS|t=-\infty} \]  \hspace{1cm} (1.62)

which shows that field configurations with \( Q_T \neq 0 \) connect different topological vacua.

In perturbation theory, one deals with zero-point quantum-mechanical fluctuations of the YM fields near one of the minima, say at \( N_\nu = 0 \). The non-linearity of the YM theory is taken into account as a perturbation and results in a series in \( g^2 \) where \( g \) is the gauge coupling. In this approach, one is apparently missing a possibility for the system to tunnel to another minima, say \( N_\nu = 1 \). The tunneling is a typical non-perturbative effect, and the instanton has a direct relation to tunneling effects.

By analogy to the double-well potential problem, the instanton solution can
be written using the 't Hooft symbol $\eta_{\mu\nu}$.

\[
\eta_{\mu\nu} = \begin{cases} 
\epsilon_{\mu\nu} & \mu, \nu = 1, 2, 3 \\
\delta_{\mu\nu} & \nu = 4 \\
-\delta_{\mu\nu} & \mu = 4 
\end{cases} \tag{1.63}
\]

and $\bar{\eta}_{\mu\nu}$ is defined by changing the sign of the last two equation. For further properties of the 't Hooft symbol, see [70]. We look for a solution of the self-dual equation in the following form analogous to the double-well potential problem:

\[
A^a_\mu = 2\bar{\eta}_{\mu\nu}^a \frac{\epsilon^{\rho\sigma} \Phi(x^2)}{x^2} \tag{1.64}
\]

where $\Phi$ has to satisfy the boundary condition $\Phi \to 0$ as $x \to \infty$. Inserting the above equation in (1.58), we find the Belavin-Polyakov-Schwartz-Tyupkin instanton solution [68].

\[
A^a_\mu(x) = \frac{2\bar{\eta}_{\mu\nu}^a \rho^2}{x^2(x^2 + \rho^2)} \tag{1.65}
\]

where $\rho$ is an arbitrary parameter characterizing the size of the instanton. The above equation describes the field of the instanton in the singular Lorentz gauge. the singularity of $A_\mu$ at $x^2 = 0$ is a gauge artifact (not physical), and the field strength and topological charge density are smooth at origin. The anti-instanton solution (with topological charge $Q = -1$) can be obtained by replacing $\bar{\eta}_{\mu\nu}^a$ with $\eta_{\mu\nu}^a$.

Inserting the above instanton solution into (1.56), we find $S = (8\pi^2|Q_T|)/g^2$. which is scale invariant and independent of instanton size $\rho$. The above action implies that in the singular gauge the tunneling probability is $P_{\text{tunneling}} = e^{-8\pi^2/g^2}$.

For the instanton solution (1.65), one can obviously shift the position of
the instanton to an arbitrary spacetime $z_\mu$ without changing the action. We can also rotate the instanton field in colour space by constant unitary matrices $U$. For $SU(N_C)$ the rotation is characterized by the total $N_C^2 - 1$ number of generators minus the $(N_C - 2)^2$ (the number of generators which do not affect the left upper $2 \times 2$ corner where the standard $SU(2)$ instanton (1.65) is residing), that is $4N_C - 5$. These degrees of freedom are called the instanton orientation in colour space. In total there are \[ [73],

$$4(\text{center}) + 1(\text{size}) + (4N_C - 5)(\text{orientations}) = 4N_C. \quad (1.66)$$

so-called collective coordinates describing the field of instantons.

### 1.3.7 Fermions in Instanton Fields

In the presence of light fermions, one can determine the fermion propagator in terms of the eigenfunctions of the Dirac operator \[ i \mathcal{D} \psi_\lambda = \lambda \psi_\lambda \].

$$S(x, y) = \sum_\lambda \frac{\psi_\lambda^*(x) \psi_\lambda^*(y)}{\lambda} \quad (1.67)$$

The crucial property of the instanton, originally discovered by 't Hooft [70], is that the Dirac operator has a zero mode \[ i \mathcal{D} \psi_0(x) = 0 \] in the instanton field. For an instanton in the singular gauge, the zero-mode wave function is

$$\psi_0(x) = \frac{\rho}{\pi (x^2 + \rho^2)^{3/2}} \frac{\gamma \cdot x}{2} \frac{1 - \gamma_3}{2} \phi \quad (1.68)$$

where \( \phi^{am} = \epsilon^{am} / \sqrt{2} \) is a constant spinor in which the $SU(2)$ colour index $\alpha$ is coupled to the spin index $m = 1, 2$.

The important properties of instantons are that each instanton (anti-instanton) has only one zero-mode. Every instanton contributes one unit to the topologi-
cal charge $Q_T = 1$ and has a left-handed zero-mode, while anti-instantons have $Q_T = -1$ and contribute a right-hand zero mode.

Now let us show how the tunneling between topologically different configurations (described semiclassically by instantons) explains the axial anomaly (i.e. the $U(1)$ puzzle). The axial anomaly can be described by (1.45)

$$\partial_\mu J^5_\mu = \frac{N_f}{16\pi^2} F^{a\mu} F^a_{\mu\nu} \tag{1.49}$$

where $N_f$ is the flavour degree of freedom. The anomaly means that loop diagrams involving external vector and axial-vector current can not be regulated in such a way that all the currents remained conserved. The change in axial charge is

$$\Delta Q_5 = Q_5(t = \infty) - Q_5(t = -\infty) = \int d^4x \partial_\mu J^5_\mu \tag{1.70}$$

In terms of the fermion propagator, $\Delta Q_5$ is given by:

$$\Delta Q_5 = \int d^4x N_f \partial_\mu Tr(S(x) x) \gamma_\mu \gamma_5$$

$$= N_f \int d^4x Tr \left( \sum_\lambda \frac{\gamma_\lambda \gamma_5 \gamma_\lambda}{\lambda} 2\lambda \gamma_5 \right) \tag{1.71}$$

For every non-zero $\lambda$, $\gamma_5 \psi_\lambda$ is an eigenvector with eigenvalue $-\lambda$. But this means that $\psi_\lambda$ and $\gamma_5 \psi_\lambda$ are orthogonal, so only zero modes can contribute to (1.71):

$$\Delta Q_5 = 2N_f (n_L - n_R) \tag{1.72}$$

Integrating the anomaly equation (1.45), we find the $\Delta Q_5$ is related to the topological charge, and the unconserved axial charge is proportional to the
instanton number \((n_L)\) minus the anti-instanton number \((n_R)\).

Thus with the help of instantons, we can understand the large \(\eta'\) mass quantitatively.

1.3.8 QCD Vacuum Structure in Instanton Background

The next natural question is the QCD vacuum structure in the instanton background. In order to assess the importance of instantons in the QCD vacuum, two crucial values have to be determined: the instanton density and the instanton size.

The tunneling rate (the instanton density, which tells how often the tunneling events happen) is determined by the standard gluon condensate from the QCD sum rules. The determination follows the idea that the non-perturbative fields contributing to the gluon condensates are dominated by the (weakly interacting) instantons. the condensate is simply proportional to the instanton density as seen in (1.56), because every single instanton contributes a finite amount.

\[
\int d^4x (F_{\mu\nu}^a)^2 = 32\pi^2
\]

If we assume that the average separations of instantons are larger than their average size (to be justified below), we can estimate the total action of the ensemble as the sum of individual action

\[
\langle G_{\mu\nu}^2 \rangle V = \int d^4x G_{\mu\nu}^2 \sim N \cdot 32\pi^2
\]

\[
\Rightarrow n = \frac{N}{V} = \frac{1}{32\pi^2} \langle G^2 \rangle \equiv \frac{1}{R^4}
\]

Inserting the gluon condensate's estimated value, we get the instanton density

54
\[ n \simeq 1 \text{ fm}^{-4}, \quad \hat{R} \simeq \frac{1}{200\text{MeV}} = 1 \text{ fm} \]  \hspace{1cm} (1.73)

Next to the instanton density, the typical instanton size is the most important parameter characterizing the instanton ensemble (the QCD vacuum structures). If instantons are too large (instantons are heavily overlapped), it doesn’t make any sense to speak of individual tunneling events, and semiclassical theory is inapplicable. If instantons are too small, then semiclassical theory is good but the tunneling rate is strongly suppressed. First by Shifman (1979) [34] and then by Shuryak (1982) [67], based on the above estimated instanton density value \((n = 1\text{ fm})\), the average size of instantons is given by

\[ \rho_e = \frac{1}{600\text{MeV}} \simeq \frac{1}{3} \text{ fm} \]  \hspace{1cm} (1.76)

with an upper limit of \(1/(500\text{ MeV})\).

With the above two values \((n \approx 1 \text{ fm}^{-4}, \rho_e \approx 1/3 \text{ fm})\), we conclude that the QCD vacuum is a dilute liquid instanton ensemble model with the following characteristics [67]:

1. Since the instanton size is significantly small than the typical separation \(R\) between instantons, \(\rho/R \sim 1/3\), the vacuum is fairly dilute.

2. The fields inside the instanton are very strong, \(G_{\mu\nu} \gg \Lambda^2\). this means that the semiclassical approximation is valid, and the typical action is large \(S_0 = 8\pi^2/g^2(\rho) \sim 10 - 15 \gg 1\) [63].

3. Instantons retain their individuality and are not destroyed by interactions [63].
The dilute liquid instanton model is strongly supported by lattice simulations [74, 75] and the agreement with the experimental results is quite impressive.

The average instanton size determines the structure of chiral symmetry breaking, in particular the value of the quark condensate and the pion mass. Now we show how instantons solve the third puzzle we posed before.

In the presence of light quarks (quark condensate problem) one has to deal with the much more complicated problem of quark-induced interactions and has to be a collective effect involving infinitely many instantons. This effect is most easily understood in the context of the mean-field method [63, 67, 73].

The light quark propagator in the mean-field approximation can be most easily derived from the effective partition function [67]. The quark gains an effective mass $M(p)$ which depends on the momentum $p$. At zero momentum, the effective quark mass (the constituent mass) is given by $M(0) \approx 350 \text{ MeV}$ [40, 73]. If we replace the current mass by the effective mass in the quark propagator, the contribution of a single instanton is given by $1/M(0)$. For a finite density of instantons, we expect:

$$
\langle \bar{q}q \rangle = i \int \frac{d^4p}{(2\pi)^4} \text{Tr} S(p) = -4N_c \int \frac{d^4p}{(2\pi)^4} \frac{M(p)}{p^2 + M(p)^2} \\
\approx -\frac{N/V}{M(0)} \approx -250 \text{ MeV}^3
$$

Both numbers $M(0)$ and $\langle \bar{q}q \rangle$ appear to be close to their phenomenological values [63].

In the QCD ground state, chiral symmetry is broken. The order parameter is the above quark condensate. The presence of a quark condensate implies that quarks can propagate over long distance. Let us explain this in a little bit more detail. When instantons interact through fermion exchanges, zero modes can become delocalized, forming a collective quark condensate. A crude picture
of quark motion in the vacuum can then be formulated as follows: instantons act as a potential well, in which light quarks can form ground states (zero modes). If instantons form an interacting liquid, quarks can travel over large distances by hopping from one instanton to another, similar to electrons in a conductor. Just as the conductivity is determined by the density of states near the Fermi surface, the quark condensate is given by the density of eigenstates of the Dirac operator near zero virtuality. If the distribution of instantons in the QCD vacuum is sufficiently random, there is a nonzero density of eigenvalues near zero, and chiral symmetry is broken.

The quantum numbers of the zero modes produce very specific correlations between quarks. First, since there is exactly one zero mode per flavour, quarks with different flavours can travel together, but quarks with the same flavour cannot. Furthermore, since zero modes have a different chirality (left-handed for instantons, right-hand for anti-instantons), quarks flip their chirality as they pass through an instanton. This is very important phenomenologically because it distinguishes instanton effects from perturbative interactions, in which the chirality of a massless quark does not change. It also implies that quarks can only be exchanged between instantons of opposite charge [63].

It is amusing that the physics of the spontaneous breaking of chiral symmetry resembles the so-called Mott-Anderson conductivity in disordered solid-state systems. Imagine random impurities (atoms) spread over a sample with finite density, such that each atom has a localized bound state for an electron. Due to the overlap of these localized electron states belonging to individual atoms, the levels are split into a band, and the electrons become delocalized, leading to conductivity of the sample. In our case the localized quark zero modes of individual instantons randomly spread over the volume get delocalized due to their overlap, which means chiral symmetry breaking [73].
In summary, we find that instantons influence the correlation function as simultaneous scattering of quarks and anti-quarks on the same instanton, leading to certain effective quark interactions. These interactions are strongly dependent on the quark-antiquark quantum numbers: they are strong and attractive in the scalar and especially in the pseudoscalar and axial scalar channels, and rather weak in the vector and tensor channels [76, 77].

1.3.9 Single-instanton Approximation

Another point of importance is the single-instanton approximation [76]. The main idea is that if the distance \( x - y \) is small compared with the typical instanton separation \( R \), we expect that the contribution from the instanton \( I = I_c \) closest to the points \( x \) and \( y \) will dominates over all others. One can distinguish this method from the dilute liquid approximation. In the dilute-liquid approximation, we systematically expand the correlation function in terms of the one, two, three, etc. instantons contributions. In the presence of light fermions (for \( \mathcal{N}_f > 1 \)), however, this method is useless because there is no zero-mode contribution to chirality-violating operators from any finite number of instantons [63].

For the propagator in the zero-mode zone, this implies,

\[
S(x, y) = \frac{\psi_L(x)\psi_L^\dagger(y)}{m^*} \tag{1.78}
\]

where the \( m^* \) is the mean-field effective quark mass.

As a result, the propagator in the single-instanton approximation looks like the zero-mode propagator of single instanton, but for a particle with the effective mass \( m^* \). By explicit calculation, we find the scalar and pseudoscalar (e.g. the \( \pi \) and \( \eta \)) correlators receive zero-mode contributions, and the contribution
is comparable to the OPE contributions \[77\]. This is one of the reasons why instantons effects are included in this thesis.

In summary, one finds the following important one-instanton effects:

1. The interaction is present for scalar and pseudoscalar correlators, but is absent in the vector and axial channels.

2. The sign of the corrections is opposite for scalar and pseudoscalar channels, but the magnitude of the corrections is same.

3. One-instanton corrections have opposite signs for isospin-one \((f_0)\) case and isospin-zero \((a_0)\) case correlators.

All these statements agree with phenomenological observations. These instantons help us solve the first puzzle we posed before. Because the opposite-sign contributions of single-instanton to the \(\pi\) and \(\eta'\) channels, we can understand the huge mass splitting between the two Goldstone bosons which have the identical OPE sum rules expression to all order. Due to the opposite contributions of single-instanton to the isospin-one and zero correlation functions, we can expect a significant mass split between \(f_0\) and \(a_0\) mesons.

In summary, instantons, one of the most non-trivial properties of non-Abelian gauge theories such as QCD, are the topologically non-trivial solutions of Euclidean field equations, describing the tunneling processes between different classical field configurations. The most important property of instantons is the existence of only one zero-mode solution of the equation of motion for each instanton. Roughly speaking, the phenomenological values of strong interactions strongly suggest that the QCD vacuum resembles the "instanton liquid" model, the reason is based on two crucial values of instantons: the typical instanton size \((\rho_c = \frac{1}{500} \text{ MeV})\) is about 1/3 of the average instanton separation \((R = \frac{1}{200} \text{ MeV})\). The instanton effects enter the correlation
functions in two ways: first is the light quark propagators get dressed in the instanton background, and through mean-field theory, one can calculate the effective quark mass. Secondly, in the single-instanton approximation, the interaction between light fermion and instantons strongly affects the correlators in the scalar and pseudoscalar channels while instantons effects are strongly suppressed in the vector and axial-vector channels. Instanton effects help to solve the $U(1)$ puzzle and quantitatively explain the spontaneously breaking of chiral symmetry. The single-instanton approximation provides the only known distinction between isospin-one and isospin-zero correlation functions, which helps to understand the mass splitting between the resonances in these two channels.
Chapter 2

Motivation

2.1 General Properties of Mesons

QCD is currently accepted as the correct theory for strong interactions and the quark model is one of the foundations of QCD. According to the quark model, there are a total of six quarks (i.e. six quark flavours), namely d, u, s, c, b, t. Each quark carries spin $1/2$, baryon number 1/3, and other additional quantum numbers. Conventionally, each quark is assigned positive parity and each anti-quark negative parity. Among the six quarks, the first three (u, d, s) are of ultimate importance, because they have relatively small masses and thus they are the components of almost all hadrons found so far. Table 2.1 lists some important properties of the three light quarks:

<table>
<thead>
<tr>
<th></th>
<th>u</th>
<th>d</th>
<th>s</th>
</tr>
</thead>
<tbody>
<tr>
<td>electric charge</td>
<td>2/3</td>
<td>-1/3</td>
<td>-1/3</td>
</tr>
<tr>
<td>current (bare) mass</td>
<td>4 MeV</td>
<td>7 MeV</td>
<td>150 MeV</td>
</tr>
<tr>
<td>constituent (dynamical) mass</td>
<td>350 MeV</td>
<td>350 MeV</td>
<td>350 MeV</td>
</tr>
<tr>
<td>isospin (z-component) $I_z$</td>
<td>1/2</td>
<td>-</td>
<td>0</td>
</tr>
<tr>
<td>strangeness</td>
<td>0</td>
<td>0</td>
<td>-1</td>
</tr>
</tbody>
</table>

The current mass means the bare mass which appears in the QCD Lagrangian (1.17), and its relatively small mass compared with hadronic mass scales is a good approximation of QCD chiral symmetry. In contrast to the nearly massless current mass, the constituent mass or the so-called effective mass results from spontaneous chiral symmetry breaking. The dynamical mass
depends on the momentum involved, the above listed values are obtained at zero momentum which can be roughly estimated as one half of the \( \rho \) meson mass or one third of the nucleon mass. Instantons are not the only approach to generate the dynamical quark mass. The constituent mass can also be generated from the OPE [40].

The three light quarks can be identified with three states in the fundamental representation of \( SU(3) \) by group theory (assuming \( m_u = m_d = m_t \)). Hadrons are therefore constructed as flavour \( SU(3) \) states. These connections between group theory and the hadronic spectrum were first observed by Gell-Mann, who noticed that when hadrons (of the same spin and parity) were plotted according to two nearly conserved quantum numbers certain distinct patterns appear. These two quantum numbers are the \( Z \)-component of isospin \( I_z \) and hypercharge \( Y = B + S \), where \( B \) is baryon number (1/3 for each light quark) and \( S \) is the strangeness. One of the biggest triumphs of the quark model is that almost all hadrons can be classified accordingly into meson and baryon families [50].

Mesons are bound states of a quark and an anti-quark (\( q \bar{q} \)) (the flavour of \( q \) and \( \bar{q} \) may be different because the strong interaction Hamiltonians are flavour independent). All the established baryons are apparently 3-quark (\( qqq \)) states. Hadrons are obtained by forming bound states of the fundamental representations of \( SU(3) \), i.e. quarks and antiquarks. All hadronic multiplets are identical to singlet, octet 8 and decuplet 10 irreducible representations of \( SU(3) \). Only 8 and 10 are observed for baryons because of restrictions imposed by spin \( (3 \otimes 3 \otimes 3 = 1 \oplus 8 \oplus 8 \oplus 10) \), and only 1 and 8 representations are observed for mesons \( (3 \otimes \bar{3} = 8 \oplus 1) \). For the purpose of this thesis, we are mainly concerned with mesons.

If the orbital angular momentum of the \( q \bar{q} \) state is \( L \), then the parity \( P \)
is \((-1)^{L+1}\). A state \(q\bar{q}\) of quark and its own antiquark is also an eigenstate of charge conjugation, with \(C = (-1)^{L+S}\), where the spin \(S\) is 0 or 1. Let \(J\) denote the total angular momentum. The \(L = 0\) states are the pseudoscalars \((J^P = 0^-)\) and vectors \((J^P = 1^-)\). The scalar mesons are \(L = 1\) states with \((J^P = 0^-)\). States with the same \(I, J^P\) and additive quantum numbers can mix. If they are eigenstates of charge conjugation, they must have the same value of \(C\). Thus the \(I = 0\) member of ground-state pseudoscalar octet mixes with the corresponding pseudoscalar singlet to produce the \(\eta\) and \(\eta'\), which appear as members of a nonet (the famous Goldstone nonet). Table 2.2 is a short summary of the pseudoscalar, vector and scalar channels relevant to this thesis:

Table 2.2: Suggested \(q\bar{q}\) quark-model assignments for most of the known mesons. Some assignments, especially for the \(0^{-+}\) multiplets are controversial.

<table>
<thead>
<tr>
<th>(N^{2S-1}L_J)</th>
<th>(J^{P\mp})</th>
<th>(ud, u\bar{u}, dd (I = 1))</th>
<th>(u\bar{u}, dd, s\bar{s} (I = 0))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1^1S_0)</td>
<td>(0^{-})</td>
<td>(\pi)</td>
<td>(\eta, \eta')</td>
</tr>
<tr>
<td>(1^3S_1)</td>
<td>(1^{-})</td>
<td>(\rho)</td>
<td>(\omega, \phi)</td>
</tr>
<tr>
<td>(1^1P_0)</td>
<td>(0^{-})</td>
<td>(a_0(980), a_0(1450), f_0(400 - 1200), f_0(980), f_0(1500))</td>
<td></td>
</tr>
</tbody>
</table>

### 2.2 Scalar Mesons

For the three meson families listed in Table 2.2, the pseudoscalar and vector mesons (the \(0^{-}\) and \(1^{-}\) channels) are well-established with extensive data. Careful data analysis and theoretical calculation indicate that the properties of these mesons, such as mass and decay width, can be well predicted by QCD and they can be classified as the bound states of a quark and an antiquark. In contrast, the nature of the scalar mesons is a long-standing puzzle, both from the experimental identification and from the theoretical calculation.
In principle, QCD should predict the hadron spectrum. But the number of scalar resonances found in the energy regime below 2 GeV exceeds the number of states that conventional quark model (i.e. the $q\bar{q}$ construction of scalar mesons) with the same quantum numbers can accommodate. According to the Particle Data Group [50], there exist four well established mesons in $I = 0$ channel: $f_0(400 - 1200)$ a very broad structure with width of 600-1000 MeV, $f_0(980)$, $f_0(1370)$ and $f_0(1500)$: two well-established resonances in $I = 1$ channel: $a_0(980)$ and $a_0(1450)$.

Table 2.3: PDG estimated mass and width values of scalar mesons

<table>
<thead>
<tr>
<th>Meson</th>
<th>Mass (MeV)</th>
<th>Width (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f_0(400 - 1200)$ or $\sigma$</td>
<td>400-1200</td>
<td>600-1000</td>
</tr>
<tr>
<td>$f_0(980)$</td>
<td>980±10</td>
<td>40-100</td>
</tr>
<tr>
<td>$f_0(1370)$</td>
<td>1200-1500</td>
<td>200-500</td>
</tr>
<tr>
<td>$f_0(1500)$</td>
<td>1500±10</td>
<td>112±10</td>
</tr>
<tr>
<td>$a_0(980)$</td>
<td>983.4±0.9</td>
<td>50-100</td>
</tr>
<tr>
<td>$a_0(1450)$</td>
<td>1474±19</td>
<td>265±13</td>
</tr>
</tbody>
</table>

In addition to the conventional light quark $q\bar{q}$ interpretation of scalar meson, there are some other candidates for the scalar meson’s structure: glueballs, hybrid mesons and multiquark-states ($qq\bar{q}\bar{q}$ or $q\bar{q} - q\bar{q}$).

The existence of gluon self-interactions in QCD suggests that additional bound states of gluons (the so-called glueball $GG, GGG$) should in principle exist. Theoretical calculations based on lattice gauge theory and QCD sum rules agree that lightest glueball should be a scalar resonance ($J^{PC} = 0^{--}$) with a mass of $1600 \pm 150 MeV$ [79, 80, 81].

Hybrid mesons are $q\bar{q}$ states combined with a gluonic excitation ($qqG$), and hence exotic (non-$q\bar{q}$) quantum numbers are allowed in this interpretation. The lightest hybrid mesons are expected in the 1500-2000 MeV mass range in flux tube models [82].
Multi-quark states might exist as a color-singlet configuration of four or more quarks. A four-quark state can be either baglike \((qq\bar{q}\bar{q})\) \([83]\), or a mesonic molecule originating from a meson-meson bound state \((qq - q\bar{q})\) \([84]\). The molecule model is more important phenomenologically, and is accepted by a large population of the high-energy physics family. Below the 2 GeV mass regime, there are several bound-state thresholds that might be interpreted as the scalar meson resonances with molecule structure. The \(KK\) threshold is about 990 MeV, therefore the \(f_0(980)\) and \(a_0(980)\) might be interpreted as \(KK\) molecules. The \(\omega\omega\) and \(\rho\rho\) thresholds are around 1500 MeV, thus the \(f_0(1500)\) and \(a_0(1450)\) might be interpreted as the combination of \(\rho\rho\) and \(\omega\omega\) molecules.

In the following, we list the possible controversial interpretations for scalar mesons, each of the interpretations has its own support from the literature.

1. \(f_0(980)\) and \(a_0(980)\) are \(qq\) quark model admixtures with \(KK\), \(\eta\pi\) and \(\eta'\pi\) continuum states \([85]\). The nearness of the \(f_0(980)\) and \(a_0(980)\) to a \(KK\) threshold has lead to a widely interpretation of \(KK\)-molecule structure \([84, 86]\), as opposed to light \(q\bar{q}\)-resonances (linear combinations of \(u\bar{u}\) and \(d\bar{d}\) states) \([41]\). However, the assumption that these states are \(KK\)-molecules have been subject to recent scrutiny. In particular, Morgan and Pennington \([87]\) have disputed the \(KK\) interpretation of \(f_0(980)\). An analysis of \(\pi\pi\) scattering \([88]\) is compatible with \(KK\) interpretation of \(f_0(980)\), but sees \(a_0(980)\) as a dynamical threshold effect, as opposed to a true resonance state. An even more recent analysis of OPAL data \([89]\) supports the consistency of a \(q\bar{q}\) interpretation of \(f_0(980)\).

2. The conventional interpretation of \(a_0(1450)\) and \(f_0(1500)\) is the quark model \((qq)\) with instanton induced interaction \([90]\). Others interpretations of these states are the lowest scalar glueball \([79, 81]\) or the bound
states of $\rho\rho, \omega\omega$ [50]. On the other hand, Lee and Weingarten [91] interpret the $f_0(1500)$ as a mainly $s\bar{s}$ state which mixes strongly with the close-by scalar glueball which show up as a resonance at 1710 MeV.

3. The more controversial state is the $\sigma$ meson ($f_0(400 - 1200)$), because of its large width (600-1000 MeV). Recent activity [92, 93, 94, 95] in reanalyzing old $\pi\pi$ and $\pi N$ scattering data has lead to the reinstatement of the lowest-lying $I = 0$ scalar resonance that is distinct from the $f_0(980)$, conservatively labeled by the 1996 and 1998 Particle Data Group [30] as $f_0(400 - 1200)$.

Moreover, the $f_0(400 - 1200)$ has been widely interpreted to be the $\sigma$ particle signature of the chiral symmetry breaking anticipated from Nambu Jona-Lasinio (NJL) dynamics [96, 97], and the linear sigma-model ($L\sigma M$) spectrum [98, 99]. Of equal importance, a clarification of the properties, or even the existence of a light $\sigma$-resonance is required to distinguish between $L\sigma M$ and $NL\sigma M$ (nonlinear sigma model) alternatives for effective theories of low-energy hadron physics [100].

In this thesis, we employ QCD Laplace sum-rules as a technique particularly well suited to relate the field theoretical content of QCD to lowest-lying resonance properties. Single-instanton effects are also included as necessary to distinguish the $I = 0$ and $I = 1$ channels' total QCD perturbative and non-perturbative effects. Another unique feature of this research is the study of finite width effects (beyond the traditional SVZ delta function resonance) in the hadronic model which is necessary in dealing with the possibly large width of the $\sigma$ meson (the finite width effects will be discussed later). With all these ideas, we try to answer the following questions:

- For the $I = 1$ channel, which of the two resonances $a_0(980)$ and $a_0(1450)$
can be identified by our QCD sum-rule method as the lowest-lying resonances with the light $q\bar{q}$ interpretation? In particular, can we rule out all but exotic interpretations of $a_0(980)$, and does there exist sum-rule support for the recently confirmed $a_0(1450)$ being the lowest-lying $qq$ object in this channel?

- For the $I = 0$ channel, which of the four candidates [$f_0(400-1200)$, $f_0(980)$, $f_0(1370)$ and $f_0(1500)$] can be interpreted as the lowest-lying resonance coupling to the light quark current (1.33)? If the existence of a $\sigma$ particle ($f_0(400-1200)$) is consistent with our QCD sum-rule analysis, is such a $\sigma$ meson a broad object, or a relatively narrower strong coupling dilaton [101]?

To conclude, the understanding of the 0-$^-$ scalar mesons is important since the determination of the lowest-lying $q\bar{q}$ interpretation states in $I = 0$ and $I = 1$ channels is of genuine value as a test of our present understanding of QCD, particular its non-perturbative content. Such lowest-lying states, when first compared with QCD via sum rules methods [42] were necessarily found to be degenerate, as purely perturbative and QCD-vacuum condensate contributions to scalar-current correlation functions cannot distinguish between $I = 0$ and $I = 1$ channels. However, the instanton component of the QCD vacuum is known to distinguish between $I = 0$ and $I = 1$ scalar states as discussed earlier (also see [102]). Such an instanton effect is quite evident in the pseudoscalar channel’s large $\pi - \eta$ mass split. Similarly, the existence of instanton solutions in QCD necessarily imposes the theoretical expectation that a similar split occurs between $I = 0$ and $I = 1$ $q\bar{q}$ scalar resonance states, with the $I = 0$ state substantially lighter than its $I = 1$ isopartner. In this regard, scalar meson spectroscopy is a genuine test of QCD.
Chapter 3

Field Theory Calculations and Hadronic Models

3.1 Perturbative Contributions

In this chapter, we calculate the perturbative expansion of the two-point scalar correlation function to two-loop level. We follow the Feynman's path integral technique as discussed in Chapter 1. First we build the full Lagrangian density $\mathcal{L}$ for QCD with the notation $\mathcal{L}_{\text{int}}$ for the interaction Lagrangian density. Then with the help of generating functional $Z \ (1.6)$, we can expand the generating functional to first order in $\mathcal{L}_{\text{int}}$ and second order in $\mathcal{L}_{\text{int}}$ respectively, corresponding to the one-loop and two-loop perturbative contributions. A critical feature of this calculation is the presence of the nontrivial feature of the renormalization constant $Z_M$ which occurs in the renormalization of the composite operator in the scalar currents.

Following the previous definition, the Lagrangian density for QCD is:

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu}^j F^{j\mu\nu} - \bar{\psi} (i \gamma^\mu D_\mu - m) \psi \quad (3.1)$$

where $D_\mu = \partial_\mu - ig \frac{\lambda}{2} A_\mu$, $g$ is the strong coupling constant, and the field strength is defined by $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + g\epsilon_{\mu\nu\lambda\kappa} A_\lambda A_\kappa$.

We can rewrite the Lagrangian density as a sum of the free Lagrangian ($\mathcal{L}_0$), and the interaction part of the Lagrangian ($\mathcal{L}_{\text{int}}$) which represents the deviations from free fields. Writing the total Lagrangian in terms of bare fields
before renormalization [26],

\[ L_{\text{total}} = -\frac{1}{2} \partial_{\mu} A^{a}_{\nu 0} (\partial_{\mu} A^{a}_{\nu 0} - \partial_{\nu} A^{a}_{\mu 0}) - \frac{1}{2a_0} (\partial_{\mu} A^{a}_{\nu 0})(\partial_{\nu} A^{a}_{\mu 0}) + \frac{i}{2} \lambda_b \partial \omega_b - m \bar{\psi}_0 \psi_0 - \frac{i}{2} (\partial^{\mu} \bar{\psi}_0) \lambda^{a} \lambda^{a} \partial_{\mu} A^{a}_{\nu 0} - \frac{1}{2} g_0 f^{abc}(\partial_{\mu} A^{b}_{\nu 0} - \partial_{\nu} A^{b}_{\mu 0})(\partial_{\mu} A^{a}_{\nu 0} - \partial_{\nu} A^{a}_{\mu 0}) + \frac{1}{2} g_0 \bar{\psi}_0 \lambda^{a} \lambda^{a} A^{a}_{\mu 0} \left( \gamma^{\mu} \right) \psi_0 = L_0 + L_{\text{int}} \] (3.2)

The interaction Lagrangian \( L_{\text{int}} \) is defined by.

\[ L_{\text{int}} = \frac{1}{2} g_0 \bar{\psi}_0 \gamma^{\mu} \lambda^{a} A^{a}_{\mu 0} \psi_0 \] (3.3)

This interaction Lagrangian contains a quark and an antiquark fields (\( \bar{\psi}, \psi \)) and a gluon field \( A^{a}_{\mu}(x) \). All interactions between quark and gluons can be derived from this Lagrangian.

Based on this observation, the interaction Lagrangian will be employed in our perturbative calculation. The generating functional, from which all Green's functions can be generated, takes the following form.

\[ Z = \int [D\psi, D\bar{\psi}, DA_{\mu}, DC, DC\bar{\psi}] e^{i \int (\bar{\psi} \gamma^{\mu} \lambda^{a} A^{a}_{\mu} \psi + \bar{\psi} \gamma^{\mu} \lambda^{a} A^{a}_{\mu 0} \psi) dz} \] (3.4)

Consider the perturbative expansion of the two-point correlation function \( \Pi(q^2) \) with the external currents:

\[ J_{I=0,1} \equiv \frac{1}{2} \left[ m_u \bar{u}(x) u(x) \pm m_d \bar{d}(x) d(x) \right] \] (3.5)

which have the same quantum numbers \( (J^{PC} = 0^{-+}) \) as the scalar mesons, the current \( J_{I=0} \) represents the isoscalar channel and \( J_{I=1} \) the isovector channel.

In the SU(2) limit, we set \( m_u = m_d = m \). The above currents correspond to
renormalization group invariant composite operators \cite{26}.

\[ m_0(\bar{\psi}_0 \psi_0)(x) = m_R(\bar{\psi}_R \psi_R)(x) \]  \hspace{2cm} (3.6)

where 0, \( R \) stand for bare and renormalized quantities. The correlator of these currents is defined as,

\[ \Pi(q^2) = i \int d^4x \ e^{i g^2 \left\{ O\right\} T[J(x)J(0)]} e^{i \int L_{int} dx dx} \]  \hspace{2cm} (3.7)

In the above expression, the fermion fields \( u \) and \( d \) in the currents (1.33) and in the interaction Lagrangian \( L_{int} \) are bare fields. Under renormalization of the above correlation function, a mass renormalization constant \( Z_m \) occur to the loop order we are working (\( m_0 = mZ_m \)).

Similar to the technique utilized in the expansion of the generating functional \( Z \), we can expand the \( e^{i \int L_{int} dx dx} \) in the power of strong coupling constant \( g \). From (3.3) we know \( L_{int} \sim g \), therefore we can also expand the exponential part in terms of \( L_{int} \) correspondingly.

\[ e^{i \int d^4x L_{int}} \sim \left( 1 + i \int d^4x L_{int} + \frac{i^2}{2} \left( \int d^4x L_{int} \right) \left( \int d^4x L_{int} \right) + \ldots \right) \]  \hspace{2cm} (3.8)

The lowest order term in \( g \) is 1 (unit) corresponding to the one loop perturbative contribution and the 2-\( L_{int} \) term the two-loop perturbative contribution.
3.1.1 One-loop Contributions with Mass Renormalization Effects

Let us start from the one-loop calculation.

\[
\Pi(q^2)_{t=0.1} = i \int d^4x \ e^{i\not{q}x} \langle O|T[J(x)] J(0)\rangle |O\rangle
\]

\[
= i \int d^4x \ \frac{m^2}{4} e^{i\not{q}x} \langle O|T[\bar{u}(x) u(x)] |O\rangle
\]

\[
\pm \bar{d}(x)d(x)\bar{u}(0)u(0) \pm \bar{d}(0)d(0)|\rangle |O\rangle
\]

(3.9)

To obtain a fully renormalized correlation function, we need to take into account the mass renormalization constant to ensure a final RG invariant result. Because only up to two-loop level is needed in our calculation, which corresponds to order \( \frac{\alpha_s}{\pi} \rightarrow \frac{\alpha_s^2}{4\pi^2} \), therefore, for the mass renormalization constant, only \( \frac{\alpha_s}{\pi} \) order should be kept, which corresponds to the one-loop renormalization mass constant \( Z_m \) [26]. In the \( \overline{\text{MS}} \) scheme where \( \frac{1}{\epsilon} = \frac{1}{\epsilon} - \ln(4\pi) + \gamma_E \) (\( \gamma_E = 0.577215 \cdots \) is the Euler-Gamma constant), the renormalization mass constant is.

\[
Z_m = 1 - \frac{\alpha_s}{\pi} C_2(R) \frac{1}{\epsilon} = 1 - \frac{\alpha}{\pi} \frac{1}{\epsilon}
\]

(3.10)

here \( C_2(R) = 4/3 \) for \( \text{SU}(3) \).

Equation (3.9) is easy to reduce to products of free field propagators through the Wick theorem [28, 45]. In conventional condensate-free perturbation theory, normal-ordered terms come from the Wick expansion annihilating the vacuum. Keep in mind that only quarks of the same flavor can form normal-ordered terms. We have

\[
\Pi(q^2)_{t=0.1} = \frac{i m^2}{4} \int d^4x \ e^{i\not{q}x} \left[ \langle O|T[\bar{u}(x) u(0)]|O\rangle \langle O|T[\bar{u}(x) u(0)]|O\rangle \right]
\]

\[
+ \ (u \rightarrow d)
\]

(3.11)
Note both $I = 0, 1$ channels give the identical expression in the lowest order perturbative calculation. Recall the free quark propagator.

\[
\langle O| T \left[ \psi_A^\dagger(x) \bar{\psi}_B^\dagger(y) \right] |O \rangle = i \delta_{\alpha \beta} \delta_{AB} S^A_\eta(x - y) \\
= i \delta_{\alpha \beta} \delta_{AB} \int \frac{d^4p}{(2\pi)^4} S^A_\eta(p) e^{-ip(x-y)} \quad (3.12)
\]

\[
S^A(p) = \frac{1}{\not{p} - m_A + i\epsilon} \quad (3.13)
\]

where $\Lambda$, $B$ are flavour indices and $\alpha$, $\beta$ colour indices.

In the above Wick expansion, only connected diagrams contribute to the perturbative correlator, so there is no combination such as $\langle O| T[\bar{u}(x)u(x)]|O \rangle$ or $\langle O| T[\bar{u}(0)u(0)]|O \rangle$ which give the annihilation diagrams.

Note also that Wick combination is always from quark point to antiquark. thus the above Wick expansion in (3.11) takes the following form.

\[
\langle O| T[\bar{u}(x_1)u(x_2)]|O \rangle \langle O| T[u(x_3)\bar{u}(x_3)]|O \rangle = Tr[(iS_F)_{23} \cdot (-iS_F)_{41}] = (S_F \cdot S_F) \quad (3.14)
\]

Perturbative calculation implies that the momentum involved is large, so it is safe to assume $p^2 \gg m^2$ and we can omit the quark mass in equation (3.13) to leading order in the chiral limit. Summing over three color indices, and remembering both $u$ quark and $d$ quark give the same contribution [$S^u(p) = S^d(p)$], we have.

\[
\Pi(q^2) = \frac{im^2}{4} \times 2_{(u-d)} \times 3_{\text{color}} \times \int \frac{d^4p}{(2\pi)^4} Tr[S(p)S(p)] \\
= \frac{i3m^2}{2} \int \frac{d^4p}{(2\pi)^4} Tr \left[ \frac{\not{p} + \not{q}}{p^2 (p + q)^2} \right] \quad (3.15)
\]
Figure 3.1: One-loop contributions to the scalar correlation function $\Pi(q^2)$. The injected current carries a momentum of $q^2$. The $u$ quark and $d$ quark give the same contribution.

The above equation corresponds to Figure 3.1.

Employing the trace identity $Tr[-\gamma^\mu \gamma^\nu] = Dg^{\mu\nu}$, we have,

$$\Pi(q^2) = \frac{i\beta m^2}{2} \int \frac{d^4p}{(4\pi)^4} \frac{D(p \cdot q + q^2)}{p^2(p + q)^2}$$  \hspace{1cm} (3.16)

From here, the dimension-regulation scheme as discussed in the previous chapters should be employed. We change our integration dimension from 4 to $D = 4 + 2\epsilon$. At the end of our calculation, we set the $\epsilon$ back to zero (back to four-dimension reality). In order to keep the coupling constant of the correlation function dimensionless, an artificial mass scale $\nu$ is introduced:

$$\int \frac{d^4p}{(2\pi)^4} \rightarrow \frac{1}{\nu^{2\epsilon}} \int \frac{d^Dp}{(2\pi)^D}$$  \hspace{1cm} (3.17)

Using the identity $p \cdot q = ((p + q)^2 - p^2 - q^2)/2$, the above equation becomes.

$$\Pi(q^2) = \frac{i\beta m^2}{\nu^{2\epsilon}} \int \frac{d^Dp}{(2\pi)^D} \left( \frac{q^2}{(p + q)^2p^2} - \frac{1}{p^2} - \frac{1}{(p + q)^2} \right)$$  \hspace{1cm} (3.18)

The resulting integrals are tabulated in [26]. we have:

$$\frac{1}{\nu^{2\epsilon}} \int \frac{d^Dp}{(2\pi)^D} \frac{1}{(p + q)^2} = \frac{1}{\nu^{2\epsilon}} \int \frac{d^Dp}{(2\pi)^D} \frac{1}{q^2} \equiv 0$$  \hspace{1cm} (3.19)
\[
\frac{1}{\nu^{2\epsilon}} \int \frac{d^D p}{(2\pi)^D} \frac{q^2}{(p + q)^2} = \frac{1}{(4\pi)^2} \left( \frac{-q^2}{4\pi \nu^2} \right)^\epsilon \Gamma(1 + \epsilon) \Gamma(1 + \epsilon) \Gamma(-\epsilon) \Gamma(2 + 2\epsilon)
\]

(3.20)

where \( \Gamma \) is the gamma function. The \( \left( \frac{-q^2}{4\pi \nu^2} \right)^\epsilon \) term can be rewritten as,

\[
\left( \frac{-q^2}{4\pi \nu^2} \right)^\epsilon = e^\epsilon \ln \left( \frac{-q^2}{4\pi \nu^2} \right) = 1 + \epsilon \ln \left( \frac{-q^2}{4\pi \nu^2} \right) + \left( \frac{\epsilon \ln \left( \frac{-q^2}{4\pi \nu^2} \right)}{2} \right) - \ldots
\]

(3.21)

The \( \Gamma \) functions can be expanded in terms of \( 1/\epsilon \) and \( \epsilon \) in \( MS \) scheme [26]. In the final form (3.20), only the constant and \( \frac{1}{\epsilon} \) terms are kept (the reason will be discussed later in this chapter).

\[
\frac{1}{\nu^{2\epsilon}} \int \frac{d^D p}{(2\pi)^D} \frac{1}{(p + q)^2} = \frac{1}{16\pi^2} q^2 \left( \frac{1}{\epsilon} - \ln \left( -\frac{-q^2}{\nu^2} \right) - 2 \right)
\]

(3.22)

Inserting this result back to (3.18), we obtain the one-loop perturbative result.

\[
\Pi(q^2)_{\text{one-loop}} = (-q^2) \frac{3m^2}{16\pi^2} \left( \frac{1}{\epsilon} - \ln \left( -\frac{-q^2}{\nu^2} \right) - 2 \right)
\]

(3.23)

Now taking the mass renormalization constant \( Z_m \) into account, which means \( m_0^2 \to m^2 Z_M^2 \), we obtain the one-loop plus the renormalization effect result.

\[
\Pi(q^2)_{\text{one-loop}}^R = (-q^2) \frac{3m^2 Z_M^2}{16\pi^2} \left( \frac{1}{\epsilon} - \ln \left( -\frac{-q^2}{\nu^2} \right) + 2 \right)
\]

(3.24)

\[
\Pi(q^2)_{\text{one-loop}}^R = (-q^2) \frac{3m^2 Z_M^2}{16\pi^2} \left( \frac{1}{\epsilon} - \ln \left( -\frac{-q^2}{\nu^2} \right) - 2 \right) \times \left( 1 - \frac{\alpha}{\pi} \frac{1}{\epsilon} \right)^2

\[
\Pi(q^2)_{\text{one-loop}}^R = (-q^2) \frac{3m^2 Z_M^2}{16\pi^2} \ln \left( -\frac{-q^2}{\nu^2} \right) \left( 1 + \frac{\alpha}{\pi} \ln \left( -\frac{-q^2}{\nu^2} \right) - 4 \right) + \frac{6}{\epsilon}
\]

Notice here we just keep the terms proportional to \( \ln \left( -\frac{-q^2}{\nu^2} \right) \), because they
are the only relevant terms which will survive after the Borel-transformation. Other possible terms in the above equation such as terms proportion to $q^2$ will disappear after Borel-transformation. The terms proportional to $\frac{1}{M}$ will be absorbed in the procedure of regulation (\(\overline{MS}\) scheme).

### 3.1.2 Two-loop Contributions

For the two-loop effects, we keep the two $\mathcal{L}_{\text{int}}$ terms in the expansion of $e^{i\int \mathcal{L}_{\text{int}}}$ in (3.8), working in the SU(2) limit ($m_u = m_d = m$).

$$
\Pi(q^2)_{I=0,1} = i \int d^4x\,d^4y\,d^4z\,\text{e}^{-i q \cdot z} \cdot \frac{i}{2} \mathcal{L}_{\text{int}}(y) \mathcal{L}_{\text{int}}(z) (O) \cdot T(J(x) J(y) J(z))
$$

(3.25)

$$
\Pi(q^2)_{I=0,1} = \frac{-i m^2}{2} \int d^4x\,d^4y\,d^4z\,e^{i q \cdot z} \\
\left( (O|T[\bar{u}_m(x)u_{n_1}(x)\bar{u}_{n_k}(0)u_{n_l}(0)]) \right) \\
\left( \frac{1}{2} g\bar{u}_m(y)(\lambda^a)_{\gamma\gamma}(\gamma^\dagger)_{\gamma\gamma} u_{n_l}(0) \right) \\
\left( \frac{1}{2} g\bar{u}_m(y)(\lambda^a)_{\gamma\gamma}(\gamma^\dagger)_{\gamma\gamma} u_{n_l}(0) \right) \\
\left( \frac{1}{2} g\bar{u}_m(z)(\lambda^a)_{\gamma\gamma}(\gamma^\dagger)_{\gamma\gamma} u_{n_l}(z) \right)
$$

(3.26)

Again we find up to two-loop level, both the $I = 0$ and $I = 1$ channels give identical results in perturbative calculation. Applying Wick's theorem and keep in mind that all quark and antiquark combination is always pointed from quark to antiquark. In the SU(2) limit, u quark and d quark give equal contributions.
Figure 3.2: Two-loop perturbative contributions to the scalar correlation function $\Pi(q^2)$. The injected current carries a momentum of $q^2$. Only connected diagrams contribute.

to the correlator.

$$\Pi(q^2)_{\text{two-loop}} = \frac{-i m^2 q^2}{16} \int d^4 x \, d^4 y \, d^4 z \left(\lambda^a\right)_{\tau \nu} \left(\lambda^b\right)_{\sigma \tau} \left(\lambda^c\right)_{\nu \rho} \left(\lambda^d\right)_{\tau \sigma} \langle O | T\left[A^Central_y(x) A^{SU}_y(z)\right] | O \rangle \langle O | T\left[u_{j\nu}(0) \bar{u}_{\alpha\beta}(x)\right] | O \rangle \langle O | T\left[u_{\alpha\beta}(x) \bar{u}_{\gamma\delta}(z)\right] | O \rangle \langle O | T\left[u_{\alpha\beta}(0) \bar{u}_{\gamma\delta}(z)\right] | O \rangle \\
\langle O | T\left[u_{j\nu}(z) \bar{u}_{\alpha\beta}(y)\right] | O \rangle \langle O | T\left[u_{j\mu}(y) \bar{u}_{\alpha\beta}(x)\right] | O \rangle \langle O | T\left[u_{\alpha\beta}(x) \bar{u}_{\gamma\delta}(0)\right] | O \rangle \\
+ \langle O | T\left[u_{j\mu}(0) \bar{u}_{\alpha\beta}(z)\right] | O \rangle \langle O | T\left[u_{j\mu}(y) \bar{u}_{\alpha\beta}(x)\right] | O \rangle \langle O | T\left[u_{\alpha\beta}(x) \bar{u}_{\gamma\delta}(0)\right] | O \rangle \\
+ \langle O | T\left[u_{j\mu}(0) \bar{u}_{\alpha\beta}(y)\right] | O \rangle \langle O | T\left[u_{j\mu}(y) \bar{u}_{\alpha\beta}(x)\right] | O \rangle \langle O | T\left[u_{\alpha\beta}(x) \bar{u}_{\gamma\delta}(0)\right] | O \rangle \\
\langle O | T\left[u_{j\mu}(0) \bar{u}_{\alpha\beta}(z)\right] | O \rangle \langle O | T\left[u_{j\mu}(y) \bar{u}_{\alpha\beta}(x)\right] | O \rangle \langle O | T\left[u_{\alpha\beta}(x) \bar{u}_{\gamma\delta}(0)\right] | O \rangle \rangle \quad \text{(3.27)}$$

Note. only the combinations which give connected diagrams contribute to the perturbative contribution. The above expression corresponds to the Feynman diagrams shown in Figure 3.2.

In Figure 3.2. Diagram (1) is equivalent to Diagram (2) which give identical
results. The gluon propagator is.

\[
\langle O | T[A_\mu^a(x) A_\nu^b(y)] | O \rangle = i \delta_{ab} D_{\mu\nu}(x - y) = i \delta_{ab} \int \frac{d^4 k}{(2\pi)^4} e^{-i k \cdot (x - y)} D_{\mu\nu}(k)
\]

\[
D_{\mu\nu}(k) = \frac{1}{k^2} \left[ -g_{\mu\nu} + (1 - \xi) \frac{k_\mu k_\nu}{k^2} \right]
\]  

(3.28)

where \( \xi \) is the gauge parameter. The final result is independent of gauge parameter, which is an arbitrary number chosen to make our calculations easier.

In our case, Feynman Gauge \((\xi = 1)\) can simplify the calculations and is employed in this thesis (another commonly used gauge choice is the Landau Gauge where \( \xi = 0 \)).

By direct calculation,

\[
\lambda^a \lambda^a = \frac{16}{3} \mathbf{1}
\]

(3.29)

where \( \mathbf{1} \) is a \( 3 \times 3 \) color-space unit matrix, and hence \( Tr[\lambda^a \lambda^a] = 16 \).  

Programs have been written in REDUCE to do these lengthy two-loop calculations (see Appendix for details). Keep in mind only the terms proportional to \( ln(-q^2/\nu^2) \) are kept since they have a non-zero Borel transformation result.

The first two diagrams give the total contribution \( \Pi(q^2)_{1-2} \),

\[
\Pi(q^2)_{1-2} = \frac{-m^2 q^2 ln(-q^2/\nu^2)}{16\pi^2} \frac{\alpha}{\pi} \left[ 2 ln(-q^2/\nu^2) - 9 - \frac{2}{\epsilon} \right]
\]

(3.30)

The third diagram gives the contribution \( \Pi(q^2)_3 \)

\[
\Pi(q^2)_3 = \frac{-m^2 q^2 ln(-q^2/\nu^2)}{16\pi^2} \frac{\alpha}{\pi} \left[ -8 ln(-q^2/\nu^2) + 38 - \frac{8}{\epsilon} \right]
\]

(3.31)

Combining the above two expressions, we obtain the two-loop contribution. In
the following expression, we set $Q^2 = -q^2$.

$$
\Pi(Q^2)_{\text{two-loop}} = \Pi(Q^2)_{\text{1+2}} + \Pi(Q^2)_{\text{3}}
= \frac{m^2 Q^2 \ln(Q^2/\nu^2) \alpha}{16\pi^2} \left[ \frac{-6\ln(Q^2/\nu^2) + 27 - \frac{6\pi}{\nu}}{\tau} \right]
$$

(3.32)

3.1.3 Perturbative Contribution to $R_0$ Laplace Sum Rules

The one-loop contribution with renormalization effects plus the two-loop contribution gives the total perturbative contribution to the correlation function to two-loop order.

$$
\Pi(Q^2)^{\text{pert}} = \Pi(Q^2)^{\text{1-loop}}_{\text{one-loop}} + \Pi(Q^2)_{\text{two-loop}}
= \frac{3m^2 Q^2 \ln(Q^2/\nu^2) \alpha}{16\pi^2} \left[ 1 - \frac{17}{3} \tau - i m^2 Q^2 \nu^2 \frac{\alpha}{\tau} \right]
$$

(3.33)

The correlation function is now used in the Laplace sum-rule expression to calculate $R_0$.

$$
R_0 = \frac{1}{\pi} \int_0^{s_0} e^{-\tau s} \text{Im} \Pi(s) \, ds
$$

(3.34)

The Laplace sum-rule $R_0$ is employed due to its property of enhancement the lowest-lying resonance's contribution and exponential suppression of the possible higher energy resonance states below continuum threshold, i.e., it is least sensitive to continuum contributions. As we discussed before, the $\Pi(s)$ is analytic function of $s$ except along the positive real $s$ axis where its imaginary parts are discontinuous. In the complex $Q^2$ plane, just above and below the $s$ axis, $Q^2$ takes the following form.

$$
Q^2 = s e^{\pm\pi}
$$

(3.35)
Therefore, above the real $s$ axis $\ln(Q^2) = \ln(s) + i\pi$, below the $s$ axis $\ln(Q^2) = \ln(s) - i\pi$. Thus the discontinuity comes from.

$$\ln(Q^2) = (\ln(s) + i\pi) - (\ln(s) - i\pi) = 2i\pi$$ (3.36)

$$\ln^2(Q^2) = (\ln(s) + i\pi)^2 - (\ln(s) - i\pi)^2 = 4i\pi \ln(s)$$ (3.37)

The imaginary part of $\Pi(s)$ is defined consistent with dispersion-relation conventions:

$$2i\text{Im}\Pi(s) = \Pi(s + i\epsilon) - \Pi(s - i\epsilon)$$ (3.38)

Insert (3.36), (3.37) and (3.33) into (3.38), we have

$$\text{Im}\Pi(t) = \left(\frac{3m^2\pi t}{16\pi^2}\right) \left(\left[1 + \frac{17}{3} \frac{\alpha}{\pi}\right] - 2 \ln(t/\nu^2) \frac{\alpha}{\pi}\right)$$ (3.39)

Insert this expression into (3.34), we have

$$R_0 = \frac{1}{\pi} \int_0^{s_0} e^{-\tau t} \text{Im}\Pi(t) \, dt$$

$$= \frac{3m^2}{16\pi^2} \int_0^{s_0} t \left(\left[1 + \frac{17}{3} \frac{\alpha}{\pi}\right] e^{-\tau t} - 2 \frac{\alpha}{\pi} \ln(t/\nu^2) e^{-\tau t}\right) \, dt$$ (3.40)

The above QCD sum-rule developed from the renormalization group invariant currents (1.33) satisfies a simple renormalization group equation [103].

$$\left(\tau \frac{\partial}{\partial \tau} + 3 \frac{\partial}{\partial \alpha} + \gamma m \frac{\partial}{\partial m}\right) R_0(\tau, s_0) = 0$$ (3.41)

Upon renormalization group improvement, the mass $m$ and the coupling constant $\alpha$ are now become $\tau$ dependent. That is they becoming running mass
\( m = m(\tau) \) and running coupling constant \( \alpha = \alpha(\tau) \). The above RG equation requires a two-loop corrections to the running mass and running coupling constant as given in (1.29) and (1.31). Upon RG-improvement, the natural choice for the scale variable \( \nu^2 \) in the sum-rule is \( \nu^2 = 1/\tau \) [103].

Using MATHEMATICA, the following integrals can be calculated:

\[
\int_0^{s_0} t \, e^{-\tau t} dt = \frac{1}{\tau^2} - \frac{1 + s_0 \tau}{e^{s_0 \tau} - 1} \tag{3.42}
\]

\[
\int_0^{s_0} t \ln(t) \, e^{-\tau t} dt = \frac{-1 - e^{s_0 \tau} E_1(s_0 \tau) - \ln(s_0) - s_0 \tau \ln(s_0)}{e^{s_0 \tau} - 1} - \frac{-1 - \gamma_E - \ln(\tau)}{\tau^2} \tag{3.43}
\]

Where the \( \gamma_E \) is the Euler-Gamma constant and \( E_1 \) is the first order Exponential-Integral function. Utilizing the above results, we have the final form of perturbative contributions to \( R_0 \).

\[
R_0^{\text{pert}}(\tau) = \frac{3m^2}{16\pi^2 \tau^2} \left( 1 + \frac{17}{3} \frac{\alpha}{\pi} \right) \left[ 1 + s_0 \tau \right] e^{-s_0 \tau} \tag{3.44}
\]

\[
- 2 \frac{\alpha}{\pi} \left[ 1 - \gamma_E + e^{-s_0 \tau} + E_1(s_0 \tau) + (1 - s_0 \tau) e^{-s_0 \tau} \log(s_0 \tau) \right]
\]
3.2 QCD Condensate Contributions

In this section we calculate the non-perturbative condensate effects. The OPE correlator takes the following general form.

\[ \Pi(Q^2) = \sum_n C_n(Q^2) \langle O_n \rangle_{\text{vac}} \]  

(3.45)

where the \( C_n(Q^2) \) are the c-number functions which can be calculated in perturbative methods, the \( \langle O_n \rangle_{\text{vac}} \) are condensates which contain the non-perturbative information. Both of the \( C_n \) and \( O_n \) series are truncated to make any calculation possible. For the \( C_n \), we just keep the lowest perturbative order.

For \( \langle O_n \rangle_{\text{vac}} \), as discussed before, only five of them have significant effects on correlation functions, they are \( \langle \bar{q}q \rangle \), \( \langle \alpha G G \rangle \), \( \langle \alpha G G G \rangle \), \( \langle \bar{q} \sigma G q \rangle \) and \( \langle q \Gamma_{\mu \nu} q \Gamma_{\mu} q \rangle \). In the light-quark cases (only \( u \) and \( d \) quarks are involved), \( \langle \alpha G G \rangle \) and \( \langle \bar{q} \sigma G q \rangle \) have negligible effects on two-point correlation functions since the mixed condensate \( \langle \bar{q} \sigma G q \rangle \) and the three-gluon condensate \( \langle \alpha G G G \rangle \) only enter at order \( m/q^2 \) [42, 43]. In the scalar channels, the contributions of these two condensates are given as [26, 42, 43].

\[ \Pi(q^2)_{\bar{q} \Gamma_{\mu \nu} q \Gamma_{\mu} q} = \left( \frac{m}{2(q^2)^2} - \frac{3m^2}{2(q^2)^3} \right) \langle \bar{q} \sigma G q \rangle \]  

(3.46)

\[ \Pi(q^2)_{\alpha G G G} = \left( \frac{27m^2}{48\pi(q^2)^3} - \frac{m^2}{4\pi(q^2)} \right) \ln(-q^2/\mu^2) \langle \alpha G G G \rangle \]  

(3.47)

In the light quark cases \( m < 10\text{MeV} \), terms proportional to \( m^2 \) are negligible compared with other terms because the typical energy scale involved in QCD is \( q^2 \sim 1\text{GeV}^2 \). Therefore, the contributions of these two condensates are safely negligible compared with other uncertainties involved in QCD sum-rule
calculations.

Therefore, in $I = 0, 1$ cases, only three condensates ($\langle \bar{q}q \rangle$, $\langle \alpha G G \rangle$, and $\langle \bar{q} \Gamma_5 q \bar{q} \Gamma_5 q \rangle$) need to be taken into account in the calculation.

### 3.2.1 Quark Condensate Contributions

Let us start from the lowest non-trivial dimension (three) quark condensate $\langle \bar{q}q \rangle$. It is the order parameter of spontaneous chiral symmetry breaking. Start again from the two-point correlation function and work in $SU(2)$ limit ($m_u = m_d = m$).

\[
\Pi(q^2)_{I=0,1} = i \int d^4 x \, e^{iq \cdot x} \langle \Omega \mid T(J(x)J(0))\mid \Omega \rangle
\]  

(3.48)

where $\Omega$ is the true vacuum state after the spontaneously symmetry breaking, and the currents are defined as in (1.33). Now Wick's theorem is employed with a quark and antiquark pair uncontracted.

\[
\Pi(q^2)_{I=0,1} = \frac{im^2}{4} \int d^4 x \, e^{iq \cdot x} \left\{ \langle \Omega \mid T[\bar{u}\alpha_i(x)u_{\alpha_j}(x) \pm \bar{d}\alpha_i(x)d_{\alpha_j}(x)]\mid \Omega \rangle \right\}
\]  

(3.49)

\[
\Pi(q^2)_{I=0,1} = \frac{im^2}{4} \int d^4 x \, e^{iq \cdot x} \left\{ \langle \Omega \mid S^{\alpha_i}_{jk}(x)\langle \bar{u}\alpha_i(x)u_{\alpha_j}(0)\rangle\mid \Omega \rangle + S^{d\alpha_i}_{u}(x)\langle \bar{u}\alpha_i(0)u_{\alpha_j(x)}\rangle + (u \rightarrow d) \right\}
\]  

(3.50)

Note the quark condensate has the same contributions in the $I = 0$ and $I = 1$ channels. The above equation can be represented graphically by Figure 3.3.

The two diagrams obviously give the same contributions. Take the free
Figure 3.3: Quark condensate contributions in the scalar channels. By symmetry, the two diagrams give the same contributions.
quark propagator $S(p)$ defined in (3.12) into account and note that both $u$ quark and $d$ quark contribute identically, we have.

$$
\Pi(q^2) = -m^2 \int d^4x \int \frac{d^4p}{(2\pi)^4} e^{-i(p-q)\cdot x} \{\langle \Omega | \bar{u}_{\alpha\nu}(x)u_{\alpha\nu}(0)|\Omega \rangle S(p)\}
$$

(3.51)

Let us consider the quark condensate $\langle \Omega | \bar{q}^A_{\alpha\nu}(x)q^B_{\beta\nu}(0)|\Omega \rangle$ where $A, B$ are the flavour indices, the $\alpha, \beta$ are color indices and $i, j$ are spin indices. We expand the quark condensate expression in powers of $x^\mu$ with the understanding that only scalars can give a non-zero vacuum expectation value.

$$
\langle \Omega | \bar{q}^A_{\alpha\nu}(x)q^B_{\beta\nu}(0)|\Omega \rangle = \langle \Omega | \bar{q}^A_{\alpha\nu}(0)q^B_{\beta\nu}(0)|\Omega \rangle + x^\mu \langle \Omega | \partial_\mu \bar{q}^A_{\alpha\nu}(0)q^B_{\beta\nu}(0)|\Omega \rangle + \cdots
$$

(3.52)

For the first term in (3.52), we can define a scalar constant $E$ such that.

$$
\langle \Omega | \bar{q}^A_{\alpha\nu}(0)q^B_{\beta\nu}(0)|\Omega \rangle = \delta_{AB}\delta_{ij}\delta_{\alpha\nu} E
$$

(3.53)

Summing over color ($\alpha, \beta$) and spin ($i, j$) indices.

$$
4 \times 3 \times 3 \times \delta_{AB} E = \langle \Omega | \bar{q}^A(0)q^A(0)|\Omega \rangle \delta_{AB} \equiv \langle \bar{q}q \rangle \delta_{AB}
$$

$$
\longrightarrow E = \frac{1}{12} \langle \bar{q}q \rangle
$$

(3.54)

For the next term in the right-hand side of (3.52), however, as the derivative is an ordinary one, the vacuum expectation value is not gauge invariant while we want to relate the terms in (3.52) to the gauge invariant condensates. It is convenient to work out all the non-perturbative contributions in the fixed
point gauge or the coordinate gauge [26, 104],

\[ x^\mu A_\mu(x) = 0 \quad (3.55) \]

It has been shown that both the fixed-point gauge and covariant gauge (discussed in Chapter 1) yield the same gauge invariant gluon condensate results [105]. In other words, the gauge dependence (whether fixed-point gauge or covariant gauge is employed in the calculation) at an intermediate stage of a calculation does not affect a genuinely gauge invariant quantity such as the gluon condensate. This argument leads us to choose the most convenient gauge, fixed-point gauge, in the gluon condensate calculation.

The fixed-point gauge allows the gauge invariant contributions of the terms in (3.52) to be extracted by replacing ordinary derivatives with covariant ones. In this gauge \( A_\mu^a(x) \) can be expressed directly in terms of the field strength tensor \( F_{\mu\nu} \), namely,

\[ A_\mu^a = \int_0^1 \alpha E_{\mu\nu}^a(\alpha x) x^\nu d\alpha \quad (3.56) \]

It is easy to show that a series of ordinary derivatives can be replaced by symmetrized, covariant derivatives in the fixed-point gauge evaluated at \( x=0 \) [106, 107]:

\[ \partial_\alpha \cdots \partial_j \psi(0) = D_{\alpha} \cdots D_j \psi(0) \quad (3.57) \]

Now we can replace the normal derivative \( \partial_\mu \) by covariant derivative \( D_\mu \) in the fixed-point gauge.

\[ \langle O | (\bar{q}^A_i D_\mu)_{\alpha}(0) q^B_{\beta j}(0) | O \rangle = F \delta_{AB} \delta_{\alpha\beta} \gamma_\mu_{ij} \quad (3.58) \]
using the equation of motion.

\[ [i\gamma_\mu D_\mu - m_A]q^A(x) = 0 \]  \hspace{2cm} (3.59)

The following relation is obtained by summing of color and spin indices in the four dimensional world.

\[ F = \frac{i}{48} m_A(q^A q^A) \]  \hspace{2cm} (3.60)

Insert \( E \) and \( F \)'s expressions back to (3.52),

\[ \langle \Omega | : q^A_{\alpha i}(x)q^B_{\beta j}(0) : \rangle_{\Omega} = \frac{1}{12} \langle \bar{q}q \rangle \delta_{\alpha j} \delta_{AB} \left( \delta_{ij} + \frac{i}{4} m_L \xi \right)_{ij} + \cdots \]  \hspace{2cm} (3.61)

Insert this expression back to (3.51) and employ the technique presented in [26].

\[ \Pi(q^2) = -m^2 \int d^4x \int \frac{d^4p}{(2\pi)^4} e^{-i(p-q)\cdot x} \{ \langle \Omega | q_{\alpha i}(x)q_{\beta j}(0) | \Omega \rangle \langle \Omega | S_{ij}(p) \rangle \} \]

\[ = \frac{-m^2}{12} \delta_{AB} \delta_{\alpha j}(\bar{q}^A q^A) \left[ Tr[S(q)] - \frac{1}{D} m_A \left( -\frac{\partial}{\partial p^\mu} Tr[S(p)] \xi \right)_{\mu=i} \right] \]  \hspace{2cm} (3.62)

The free quark propagator is \( S(p) = \frac{1}{p^2 - m} \), where \( m = m_u = m_d \) is the quark mass. In the light quark cases where the energy involved in the perturbative procedure is much larger than the quark’s mass \( (\frac{m^2}{p^2} \ll 1) \), the quark mass in the denominator just contributes to \( \mathcal{O}(m) \) corrections.
Summing over color indices, we have.

\[
\Pi(q^2) = \frac{-m^2 \times 3 \times 3}{12 \times 4} \left[ \langle \bar{q}q \rangle \text{Tr}[S(q)] - \frac{m\langle \bar{q}q \rangle}{4} \left( -\frac{\partial}{\partial p^\mu} \text{Tr}[S(p) \gamma^\mu] \right)_{\mu=q} \right]
\] (3.63)

The term \(\text{Tr}[S(p)]\) gives \(\mathcal{O}(m)\) corrections. Note that the trace in the second term \(\text{Tr}[S(P) \gamma^\mu]\) still requires a color summation, and we write \(m\langle \bar{q}q \rangle\) as \(\langle m\bar{q}q \rangle\).

\[
\Pi(q^2) = \frac{-m^2 \times 3 \times 3}{12 \times 4} \langle m\bar{q}q \rangle \left[ -\frac{\partial}{\partial p^\mu} \text{Tr}[\frac{\not{p}}{p^2} \gamma^\mu] \right]_{\mu=q}
\] (3.64)

Using the identity [26]

\[
\frac{-\partial}{\partial p^\mu} S(p) = S(p) \gamma^\mu S(p)
\] (3.65)

\[
\Pi(q^2)_{\langle q\bar{q} \rangle} = \frac{-m^2 \times 3 \times 3}{12 \times 4} \langle m\bar{q}q \rangle \text{Tr} \left[ \frac{\not{p}}{p^2} \gamma^\mu \frac{\not{p}}{p^2} \gamma^\mu \right]_{\mu=q}
\]

\[
= -\frac{3m^2}{2q^2} \langle m\bar{q}q \rangle
\] (3.66)

### 3.2.2 Gluon Condensate Contributions

The next lowest-dimension condensate is the dimension four gluon condensate \(\langle \alpha_s G G \rangle\), where the \(\alpha_s\) is the strong coupling constant. Still working in the fixed-point gauge (coordinate gauge) \(x^\mu A_\mu = 0\), we expand the correlation function to the next leading order as we did for the two-loop perturbative calculation.

\[
\Pi(q^2)_{l=0.1} = i \int d^4x \, d^4y \, d^4z \, e^{i q z} \langle \Omega | \mathcal{T} \{ J(x) J(y) \} \frac{i^2}{2} \mathcal{L}_{\text{int}}(y) \mathcal{L}_{\text{int}}(z) | \Omega \rangle
\] (3.67)
where the interaction Lagrangian takes the following form.

\[ \mathcal{L}_{\text{int}} = \frac{1}{2} g \bar{\psi} \gamma^\mu \lambda^a \mathcal{A}_\mu^a \psi \]  

(3.68)

\[ \Pi(q^2)_{\ell=0,1} = \frac{-im^2}{2} \int d^4x \, d^4y \, d^4z \, \epsilon^{\mu \nu \alpha \beta} \left\{ \langle \Omega | T(\bar{\psi}_{\alpha \beta}(x) \psi_{\gamma \delta}(y)) u_{\alpha \beta}(0) \right\} \]

\[ \frac{1}{2} g \bar{\psi}_{\gamma \delta}(y) (\lambda^a)_{\gamma \delta} (\gamma^\lambda)_{\mu \nu} u_{\mu \nu}(y) \mathcal{A}_{\lambda}^a(y) \]

\[ \frac{1}{2} g \bar{\psi}_{\gamma \delta}(z) (\lambda^b)_{\epsilon \tau} (\gamma^\rho)_{\mu \nu} u_{\epsilon \tau}(z) \mathcal{A}_{\rho}^b(z) \Omega \right\} + (u \rightarrow d) \]  

(3.69)

Employing Wick's theorem and working in the SU(2) limits \( m_u = m_d = m \), leaving just one pair of \( \mathcal{A}_\mu \mathcal{A}_\nu \) non-contracted, we obtain the following expression.

\[ \Pi(q^2)_{\alpha \Gamma \Gamma} = \frac{-im^2 g^2}{16} \left( \lambda^a \right)_{\gamma \delta} \left( \lambda^b \right)_{\epsilon \tau} (\gamma^\lambda)_{\mu \nu} (\gamma^\rho)_{\mu \nu} \]

\[ \int d^4x \, d^4y \, d^4z \, \epsilon^{\mu \nu \alpha \beta} \left\{ \langle \Omega | T(\mathcal{A}_{\mu}^a(y) \mathcal{A}_{\nu}^b(z)) \mathcal{A}_{\lambda}^a(z) \mathcal{A}_{\rho}^b(z) \Omega \right\} \]

\[ S_{\mu \alpha}^a(x) S_{\nu \beta}^a| x - z | S_{\mu \alpha}^a(z - y) S_{\nu \beta}^a(y) \]

\[ + S_{\mu \alpha}^a(z) S_{\nu \beta}^a(y - z) S_{\mu \alpha}^a(y - x) S_{\nu \beta}^a(x) \]

\[ + S_{\mu \alpha}^a(y) S_{\nu \beta}^a(y - x) S_{\mu \alpha}^a(z - x) S_{\nu \beta}^a(z) \]  

(3.70)

Taking into account the quark propagator (3.12) and noting the colour algebra
Figure 3.4: Gluon condensate contributions in the scalar channels. By symmetry, the first two diagrams give the same contribution.

gives two.

\[
\Pi(q^2)^{(GG)}_{I=0,1} = \frac{-i m^2 q^2}{4} \int d^4 y d^4 z \int \frac{d^4 p_1}{(2\pi)^4} \frac{d^4 p_2}{(2\pi)^4} \frac{d^4 p_3}{(2\pi)^4} (\overline{\Omega} A_\mu^a(y) A^a_\nu(z) \Omega) \\
\left\{ Tr[S(p_1 + q)\gamma^\lambda S(p_3)\gamma^\rho S(p_2)S(p_1)] e^{i(q-p_1-p_3)\gamma^\mu(p_1-p_2)\gamma^\nu z} \\
- Tr[S(p_1)S(p_3)\gamma^\lambda S(p_2)\gamma^\rho S(p_1-q)] e^{i(q-p_1-p_3)\gamma^\mu(p_1-p_2)\gamma^\nu z} \\
+ Tr[S(p_1)\gamma^\rho S(p_2)S(p_3)\gamma^\lambda S(p_1-q)] e^{i(q-p_1-p_3)\gamma^\mu(p_1-p_2)\gamma^\nu z} \right\} 
\]  
(3.71)

Note again the gluon-condensate contributions have the same results for both \( I = 0 \) and \( I = 1 \) channels. The above expression corresponds to the diagrams in Figure 3.4.

Working in the fixed-point gauge and using the expression (3.56), we expand the gluon field in terms of covariant derivatives [26]

\[
A_\mu(x) = \sum_{n=0}^{\infty} \frac{1}{n!(n+2)} x^0 x^1 \cdots x^n \\
[D_{\omega_1}(0), [D_{\omega_2}(0), \cdots [D_{\omega_n}(0), G_{\omega\mu}(0)] \cdots ] 
\]  
(3.72)
Now the vacuum expectation value in (3.71) can be written as

\[
\langle \Omega | A_\lambda^a (y) A_\rho^a (z) | \Omega \rangle = \frac{1}{4} g^{\nu \kappa} z^\tau \langle \Omega | G^a_{\nu \lambda} G^a_{\tau \rho} (0) | \Omega \rangle + \cdots
\]

\[
= \frac{1}{4 D (D - 1)} g^{\nu \kappa} z^\tau [g_{\nu \tau} g_{\lambda \rho} - g_{\nu \rho} g_{\lambda \tau}] \langle \Omega | G^a_{\mu \nu} (0) G^a_{\mu \rho} (0) | \Omega \rangle \cdots
\]

\[
= \frac{1}{D (D - 1)} g^{\mu \nu} z^\tau [g_{\nu \tau} g_{\lambda \rho} - g_{\nu \rho} g_{\lambda \tau}] \langle GG \rangle + \cdots
\] (3.73)

Where \( D \) is the dimension we are working with. Substituting this expression back to (3.71), we obtain

\[
\Pi (q^2) = \frac{- m^2 g^2}{8 D (D - 1)} \int d^4 y d^4 z \int \frac{d^4 p_1}{(2 \pi)^4} \frac{d^4 p_2}{(2 \pi)^4} \frac{d^4 p_3}{(2 \pi)^4} (GG) [g_{\nu \tau} g_{\lambda \rho} - g_{\nu \rho} g_{\lambda \tau}] y^{\nu} z^\tau
\]

\[
\{ 2 T r [S(p_1 - q) s^\lambda S(p_3) s^\mu S(p_2) S(p_1)] e^{i(q - p_1 - p_2 - p_3) \cdot z} - T r [S(p_1) s^\mu S(p_2) S(p_1 - q)] e^{i(q - p_1 - p_2 - p_3 - p_1) \cdot z} \}
\] (3.74)

and hence

\[
\Pi (q^2) = \frac{- m^2 g^2}{8 D (D - 1)} \langle GG \rangle [g_{\nu \tau} g_{\lambda \rho} - g_{\nu \rho} g_{\lambda \tau}] \int \frac{d^4 p_1}{(2 \pi)^4} \left\{ \frac{\partial}{\partial p_{1 \nu}} \frac{\partial}{\partial p_{2 \mu}} T r [S(p_1 + q) s^\lambda S(p_3) s^\mu S(p_2) S(p_1)] \right\}_{p_2 = p_3 = p_1 - q}
\]

\[
+ \left. \frac{\partial}{\partial p_{1 \nu}} \frac{\partial}{\partial p_{2 \mu}} T r [S(p_1) s^\mu S(p_2) S(p_3) s^\lambda S(p_1 - q)] \right\}_{p_2 = p_1, p_2 = p_1 - q}
\] (3.75)

The trace calculations can be evaluated with the REDUCE program and using (3.65), the final form of the gluon condensate contribution to correlation function is

\[
\Pi (q^2)_{(aGG)} = - \frac{1}{16 q^2 \pi} (\alpha_s GG)
\] (3.76)
where the strong coupling constant $\alpha_s$ is equal $g^2/4\pi$.

In order to check the consistency of our calculations, we employ another technique, the plane wave method, to calculate the gluon-condensate contributions again. The plane-wave method begins with Wilson's operator identity [36]. After forming a vacuum expectation value of the operator relation, appropriately chosen states can be sandwiched to single out the contribution of a given operator.

By explicit calculation of the gluon condensate contribution with the help of the program REDUCE, we find the two methods give identical results, which is what we expect.

### 3.2.3 Dimension-six Condensate Contributions

The dimension six condensate $\langle O_6 \rangle$ (the four-quark condensate) can be obtained by expanding the two-point correlation function (3.26), leaving two quark-antiquark pairs uncontracted. Keeping in mind only connected diagrams must be taken into account, we find.

\[
\Pi_{O_6}(q^2) = \frac{-i m^2}{2} \int \frac{d^4x d^4y d^4z}{4} e^{i q \cdot x} \sum_{A,B,C,D} \left\{ \langle \Omega | T(\epsilon_A \bar{q}^A_{\alpha_a}(x) q^A_{\alpha_j}(x) \epsilon_B \bar{q}^B_{\alpha_b}(0) q^B_{\alpha_l}(0) \right\}
\]

\[
\frac{1}{2} g \bar{q}_{s\alpha}(y)(\lambda^a)_{s\alpha}(-\lambda^a)_{m\alpha} q_{\alpha m}(y) A_1^a(y)
\]

\[
\frac{1}{2} g \bar{q}_{s\alpha}(z)(\lambda^b)_{s\alpha}(-\lambda^b)_{s\alpha} q_{\alpha s}(z) A_1^b(z) \Omega \}
\]

\[3.77\]
where $A, B, C, D$ are flavour indices. $\epsilon_u = +1, \epsilon_d = -1$ and zero for other flavour.

$$
\Pi_{S_4}(q^2) = \frac{-i m^2 g^2}{32} (\lambda^a)_{\gamma^\delta} (\lambda^b)_{\gamma^\epsilon} (\gamma^\lambda)_{\mu\nu} (\gamma^\rho)_{st} \\
\int d^4x d^4y d^4z e^{i q \cdot x} \sum_{A, B, C, D} D_{ab}^{st}(y - z) \\
\left\{ - S_{ri}^{\alpha,CA}(y - x) S_{tk}^{\tau, DB}(z)(\Omega(q_{s_{m}r}^B(y)q_{t_{l}r}^C(z)q_{s_{l}r}^B(x)q_{t_{m}r}^C(0)))\Omega \\
+ S_{ri}^{\alpha,CA}(y - x) S_{ls}^{\tau, BD}(z)(\Omega(q_{s_{k}r}^B(0)q_{t_{l}r}^C(z)q_{s_{l}r}^B(x)q_{t_{k}r}^C(z)))\Omega \\
- S_{li}^{\alpha,BA}(x) S_{jm}^{\gamma, AC}(x - y)(\Omega(q_{s_{k}r}^B(0)q_{t_{l}r}^C(z)q_{s_{l}r}^B(y)q_{t_{m}r}^C(z)))\Omega \\
- S_{li}^{\alpha,BA}(x) S_{rk}^{\gamma, CB}(y)(\Omega(q_{s_{m}r}^B(y)q_{t_{l}r}^C(z)q_{s_{l}r}^B(x)q_{t_{m}r}^C(z)))\Omega \\
- S_{ri}^{\alpha,CA}(y - x) S_{lm}^{\gamma, BC}(y)(\Omega(q_{s_{k}r}^B(0)q_{t_{l}r}^C(z)q_{s_{l}r}^B(x)q_{t_{m}r}^C(z)))\Omega \\
+ \text{the same terms with } q \to \bar{q} \right\} \\
(3.78)
$$

Its diagrammatic representations are given in Figure (3.5). The diagrams in Figure 3.5 where quarks and antiquarks are exchanged are the same but the sense of the fermionic lines are reversed.
Figure 3.5: Dimension-six four-quark condensate contributions to the two-point correlation function in the scalar channels.
In order to deal with the four quark condensate we are going to assume the vacuum saturation hypothesis [34], i.e.

$$
\langle \Omega | \bar{q}^A(x)q^B(y)q^C(z)q^D(t)|\Omega \rangle = f_{vs}(\langle \Omega | \bar{q}^A(x)q^D(t)|\Omega \rangle \langle \Omega | q^B(z)q^C(z)|\Omega \rangle - \langle \Omega | \bar{q}^A(x)q^C(z)|\Omega \rangle \langle \Omega | q^B(z)q^D(t)|\Omega \rangle) \quad (3.79)
$$

where the $f_{vs}$ is the vacuum saturation factor. Utilizing the same techniques used before, the four-quark condensate contribution to the $\Pi(q^2)$ is given as in [26],

$$
\Pi_{\sigma_4}(q^2) = -\frac{88m_{\pi}^2}{27(q^2)^2}f_{vs}(\alpha(\bar{q}q))^2 \quad (3.80)
$$

### 3.2.4 QCD Condensate Contributions to $R_0$—Borelization

Adding equation (3.66, 3.76, 3.80) together, we obtain the QCD condensate contributions to $\Pi(Q^2)$ ($Q^2 = -q^2$).

$$
\Pi(Q^2)_{\text{cond}} = \frac{3m^2}{2Q^2} \langle m\bar{q}q \rangle + \frac{1}{16} \frac{m^2}{Q^2 \pi} \langle \alpha_s GG \rangle - \frac{88m_{\pi}^2}{27(q^2)^2}f_{vs}(\alpha(\bar{q}q))^2 \quad (3.81)
$$

As we discussed before, the QCD Laplace sum-rule $R_0(\tau, s_0)$ is used in our analysis instead of $\Pi(Q^2)$. Hence a device is needed to transfer the $\Pi(Q^2)$ expression to $R_0(\tau, s_0)$, the device we refer to is the Borelization and it consists in applying the following operator $B$ to $\Pi(Q^2)$.

$$
\hat{B}_{M^2} = \lim_{Q^2 \to \infty} \left( \frac{-Q^2}{n-1} \right)^n \left( \frac{\partial}{\partial Q^2} \right)^n \quad (3.82)
$$
where $Q^2/n \equiv M^2$. Two important Borelization identities are.

$$
\hat{B} \left( \frac{1}{Q^2} \right)^n = \frac{1}{(n-1)!} \left( \frac{1}{M^2} \right)^n \cdot \hat{B} \left( \frac{1}{s+Q^2} \right) = \frac{1}{M^2} e^{-s/M^2}
$$

(3.33)

From the above equation, we find that the advantages of Borelization are its properties of exponential suppression of large $s$ in the form of $1/(s+Q^2)$, and the factorial suppression of higher order $(1/Q^2)$ terms.

The QCD condensates part of $\Pi(Q^2)$ and $R_0(\tau, s_0)$ are related by the dispersion relation.

$$
\Pi(Q^2) = \frac{1}{\pi} \int ds \frac{I_m \Pi(s)}{s + Q^2} + \text{const}
= C_1 \frac{\langle \bar{q}q \rangle}{Q^2} + C_2 \frac{\langle \alpha GG \rangle}{Q^2} + C_3 \frac{\langle \bar{q}q\bar{q}q \rangle}{(Q^2)^2} + \text{const}
$$

(3.34)

Apply the Borel transformation.

$$
\hat{B} \Pi(Q^2) = \frac{1}{\pi} \int ds \frac{I_m \Pi(s) e^{-1/M^2}}{M^2}
= C_1 \frac{\langle \bar{q}q \rangle}{M^2} + C_2 \frac{\langle \alpha GG \rangle}{M^2} + C_3 \frac{\langle \bar{q}q\bar{q}q \rangle}{(M^2)^2}
$$

(3.35)

By definition (3.34), we find the following relation.

$$
R_0(\tau, s_0) = C_1 \langle \bar{q}q \rangle + C_2 \langle \alpha GG \rangle + C_3 \langle \bar{q}q\bar{q}q \rangle \tau
$$

(3.36)

where $1/M^2 = \tau$ is used. Inserting (3.31) into the above equation, we obtain the QCD condensate contributions to $R_0$.

$$
R_0(\tau, s_0) = \frac{3m^2}{2} \langle m\bar{q}q \rangle + \frac{1}{16} \frac{m^2}{\pi} \langle \alpha_s GG \rangle - \frac{88m^2\pi}{27} f_{rs} \langle \alpha_s (\bar{q}q)^3 \rangle \tau
$$

(3.37)
3.3 Instanton Contributions

We have discussed the instanton effects in Chapter 1 and found that it corresponds to the effects of tunneling from one local vacuum minimum to another minimum with different topological numbers. These non-perturbative effects are totally ignored in the normal perturbative mechanism of QCD. In the instanton liquid model, the light quark propagators get dressed in the instanton background and obtain the dynamical (effective) mass $m$. 73. We also emphasized that single-instanton effects are non-negligible in comparison with the OPE contributions 77. Single-instanton corrections to the two-point correlation functions have opposite signs for isospin one ($I=1$) and isospin zero ($I=0$) scalar channels. Now we perform an explicit calculation for $I=0,1$ channels and illustrate the non-negligible contribution to the corresponding correlator, and hence illustrate the importance of including instanton effects in this research.

Now let us start from the two-point correlation function using the currents defined in (1.33).

\[
\Pi(q^2)_{I=0,1} = i \int d^4 x \, d^4 y \, e^{im(x-y)} \Pi(x,y)
\]

(3.38)

\[
\Pi(x,y)_{I=0,1} = \frac{m^2}{4} \langle O | T[\bar{u}_{\alpha_1}(x)u_{\alpha_1}(x) \pm \bar{d}_{\alpha_1}(x)d_{\alpha_1}(x)]|O\rangle
\]

\[
\bar{u}_{jk}(y)u_{jl}(y) \pm \bar{d}_{jk}(y)d_{jl}(y)\rangle
\]

(3.39)

Now employing Wick's theorem, and noting that due to instanton effects, not only connected diagrams contribute, but the annihilation diagrams also contribute [76, 77]. Intuitively, we can think the single-instanton contributes to the two-point function as shown in Figure 3.6.
Figure 3.6: Single-instanton effects in the scalar correlation function resulting in both of the connected and annihilated diagrams contributing to (3.88).
Wick’s theorem takes the following form for the four-fermion ($\psi^3$) interaction in the instanton background:

$$
\langle O | T(\bar{\psi}_1 \psi_2 \bar{\psi}_3 \psi_4) | O \rangle = \langle O | (\bar{\psi}_1 \psi_2) | O \rangle \langle O | T(\bar{\psi}_3 \psi_4) | O \rangle + \langle O | T(\bar{\psi}_1 \psi_4) | O \rangle \langle O | T(\bar{\psi}_2 \psi_3) | O \rangle \\
= (-iS^F)_{21}(-iS^F)_{43} + (iS^F)_{23}(-iS^F)_{11} \\
= -S^F_{24}S^F_{31} + S^F_{23}S^F_{34} \quad (3.90)
$$

where $S^F$ is the quark propagator defined in (3.12).

Keep in mind that only quark and antiquark with the same flavour can be contracted. we find the following form of the Wick contraction for the unflavoured current components:

$$
\langle O | T[\bar{u}_{\alpha i}(x)u_{\alpha j}(x)\bar{u}_{\beta k}(y)u_{\beta l}(y)] | O \rangle \\
= Tr[S_u(x, y)S_u(y, x)] - Tr[S_u(x, x)]Tr[S_u(y, y)] \quad (3.91)
$$

For the flavoured current components.

$$
\langle O | T[\bar{u}_{\alpha i}(x)u_{\alpha j}(x)\bar{d}_{\beta k}(y)d_{\beta l}(y)] | O \rangle \\
= -Tr[S_u(x, x)]Tr[S_d(y, y)] \quad (3.92)
$$

Put these results back to (3.89). and work in the SU(2) limits ($m_u = m_d = m$. $S_u = S_d = S$).

$$
\Pi(x, y)_{t=0, 1} = \frac{m^2}{2} \left( Tr[S(x, y)S(y, x)] - Tr[S(x, x)]Tr[S(y, y)] \right) \\
\mp \frac{m^2}{2} Tr[S(x, x)]Tr[S(y, y)] \quad (3.93)
$$

Please note the $\mp$ sign in the above equation. this is the first time we find a distinction between contributions to the $I = 0, 1$ scalar current correlation.
functions (1.33). This mechanism will be responsible for the breaking of mass degeneracy between the $I = 0.1$ scalar channels.

As discussed before, for the cases involving light-quarks in the instanton background, the ’t Hooft zero-mode solution is always employed. The zero-mode light quark gains an effective mass $m_\ast$ and the zero-mode fermion propagator is [108].

$$S_\ast(x, y) = \langle O | q_\ast^a(x) q_\ast^b(y) | O \rangle = \int d^4z \frac{[\gamma^\ast_\mu(x) \gamma^\ast_\nu(y)]^{a_b}}{m_\ast}$$

which retains only the zero-mode. In the singular gauge, the zero-mode fermion solution takes the following form [70],

$$\gamma^\ast_\mu(x) = \frac{\sqrt{2} \rho}{\pi \sqrt{x^2 (x^2 + \rho^2)^{3/2}}} \chi^\ast \gamma^\ast_\mu$$

$$= \sqrt{2} \phi(x) \gamma^\ast \gamma^\ast_\mu$$

where $\chi^\ast$ is the colour-spin matrix, $\gamma^\ast_\mu$ denotes the instanton and anti-instanton contributions [70, 109].

The quantity $\phi(x)$ is defined as,

$$\phi(x) = \frac{\sqrt{2} \rho}{\pi \sqrt{x^2 (x^2 + \rho^2)^{3/2}}}$$

$$\chi^\ast \sim \gamma^\mu \frac{1 + \gamma_5}{2} \gamma^\ast_\mu \text{ } \text{ } \text{some } \text{ colour, } \text{ Dirac } \text{ column}$$

$$\chi \chi^\ast = \frac{1}{16} \left( \gamma^\mu \gamma^\nu \frac{1 \pm \gamma_5}{2} \right) \left( U^{-1} \gamma^\mu \gamma^\nu L^\dagger \right)$$

where $U \in SU(N_C)$ is the colour orientation matrix of the instanton.
tion over the instanton orientation as discussed in (1.66). we have the following
gauge averaged expression for a single instanton and anti-instanton [102, 109],

$$
\langle \chi^\pm \chi^\pm \rangle = \frac{1}{2} \left( \frac{1 \pm \gamma_5}{2} \right)
$$

(3.99)

$$
\langle [\chi^\pm \chi^\pm]_{\alpha_1, \beta_1}[\chi^\pm \chi^\pm]_{\alpha_2, \beta_2} \rangle_{\text{range}} = \frac{1}{2} \left( \frac{1 \pm \gamma_5}{2} \right)_{\beta_1, \beta_2} \left( \frac{1 \pm \gamma_5}{2} \right)_{\alpha_1, \alpha_2}
$$

(3.100)

where $\alpha_1, \alpha_2, \beta_1, \beta_2$ are Dirac indices. Using the zero-mode solution of the
fermions in the instanton background, the light quark propagator can be written as.

$$
S(x, y) = \psi_0^\dagger(x) \psi_0^\dagger(y) = 2 \phi(x) \phi(y) \not\! \psi \not\! \chi \not\! \chi \not\! \gamma \not\! \not\! \partial
$$

(3.101)

Now we can investigate the properties of the correlation functions of $I = 0, 1$
channels as defined in (3.93). Start from the first term in the right-hand side
of (3.93).

$$
Tr[S(x, y)S(y, x)] = Tr[4 \phi^2(x) \phi^2(y) \not\! \psi \not\! \chi \not\! \chi \not\! \gamma \not\! \not\! \partial \not\! \psi \not\! \chi \not\! \chi \not\! \gamma \not\! \not\! \partial
$$

$$
= 4 \phi^2(x) \phi^2(y) Tr \left[ \frac{1}{2} \not\! \psi \not\! \chi \not\! \chi \not\! \gamma \not\! \not\! \partial \not\! \psi \not\! \chi \not\! \chi \not\! \gamma \not\! \not\! \partial \right]
$$

$$
= 2 \phi^2(x) \phi^2(y) Tr \left[ \frac{1}{2} \not\! \psi \not\! \chi \not\! \chi \not\! \gamma \not\! \not\! \partial \not\! \psi \not\! \chi \not\! \chi \not\! \gamma \not\! \not\! \partial \right]
$$

(3.102)

where the trace of the four colour-spin matrices $\chi$ follows from equation (3.100).

Employing the following identities.

$$
Tr[\not\! a_1 \not\! a_2 \not\! a_3 \not\! a_4] = 4(a_1 \cdot a_2 a_3 \cdot a_4 - a_1 \cdot a_3 a_2 \cdot a_4 + a_1 \cdot a_4 a_2 \cdot a_3)
$$

(3.103)
\[ \text{Tr}[\gamma^5 \gamma^\mu \gamma^\nu \gamma^\rho] \equiv 0 \quad (3.104) \]

We find,

\[ \text{Tr}[S(x,y)S(y,x)] = 2 \times 2 \sigma^3(x) \sigma^3(y) 2x^2y^2 = 8 \sigma^3(x) \sigma^3(y)x^2y^2 \]

\[ (3.105) \]

In the above calculation, a summation of the identical contribution of single instanton and anti-instanton, which gives a factor of two, has been employed.

For the second term in (3.93),

\[
\text{Tr}[S(x,y)] \text{Tr}[S(y,x)] = \text{Tr}[2\sigma(x)\sigma(y)\frac{1}{2} \gamma^\mu \frac{\gamma^\nu + \gamma^\rho}{2} \gamma^\rho] \\
\times \text{Tr}[2\sigma(x)\sigma(y)\frac{1}{2} \gamma^\nu \frac{\gamma^\mu + \gamma^\rho}{2} \gamma^\rho] \\
= 2 \times \sigma^3(x) \sigma^3(y) 2x^2y^2 \\
= 8x^2y^2 \sigma^3(x) \sigma^3(y) \quad (3.106)
\]

where the trace of colour-spin matrices follows from (3.99) and the summation of instanton and anti-instanton contributions is included. The relations

\[ \text{Tr}[\sigma \gamma^\mu \gamma^\nu] = 4a \cdot b \text{ and } \text{Tr}[\gamma^\mu \gamma^\nu \gamma^\rho] = 0 \]

are employed.

From the above two equations (3.106) and (3.105), we can conclude that,

\[ \text{Tr}[S(x,y)S(y,x)] = \text{Tr}[S(x,x)] \text{Tr}[S(y,y)] \quad (3.107) \]

Inserting this result back to (3.93), we have

\[ \Pi_{I=1,0}(x,y) = \frac{m^2}{2} \text{Tr}[S(x,x)] \text{Tr}[S(y,y)] \quad (3.108) \]

To this end, we have proved that the instanton contributes oppositely to isospin
one and isospin zero channels with the same magnitude.

Note an important property of the above equation is that effectively only the
annihilation parts of the two-point function contribute to the single instanton
correlator.

It is interesting to illustrate the different roles the instanton and perturba-
tive QCD played in the two-point function $\Pi(x, y)$.

\[
\Pi_{I=0,1}(x, y) = \langle O | T [\bar{u}(x) u(x) \pm \bar{d}(x) d(x)] [\bar{u}(y) u(y) \pm \bar{d}(y) d(y)] | O \rangle
\]
\[
= \langle O | T [\bar{u}(x) u(x) \bar{u}(y) u(y) + \bar{d}(x) d(x) \bar{d}(y) d(y)] | O \rangle
\]
\[
= \langle O | T [\bar{u}(x) u(x) \bar{d}(y) d(y)] | O \rangle
\]
\[
= \langle O | T [\bar{u}(y) u(y) \bar{d}(x) d(x)] | O \rangle
\]

In perturbative QCD approach, only the first term in the right-hand side of
above equation contributes, while the other terms vanish identically due to
their annihilation properties. In the single instanton background approach, as
seen from (3.107), the first term in the right-hand side is canceled by one of
the remaining terms. Therefore, only one of the remaining annihilation terms
gives the instanton contribution but with an opposite sign for spin one and
spin zero channels. In this way, the instanton effects are responsible for the
mass splitting between the lowest-lying resonances in $I = 0.1$ channels.

Now let us calculate the instanton effects in $I = 0$ channels as an example.

\[
\Pi_{I=0}(x, y) = -\frac{m^4}{2} Tr[S(x, x) | Tr[S(y, y)]
\]
\[
= -4m^4 \sigma^2(x) \sigma^2(y) x^2 y^2
\]
where the result from (3.105) is used.

\[
\Pi(q^2) = \int d^4x_0 \int d^4x \int d^4y \, e^{i q \cdot (x-x_0)} \, \rho \phi^2(y-x_0) \Pi(x, y)
\]

(3.111)

and \(x_0\) is the instanton’s position. Additionally, as discussed in Chapter 1, an integral over the instanton density \(n_r(\rho) = n_c \delta(\rho - \rho_c)\), \(\rho_c = 1/(600 \, M \, V^{-1})\) must be performed. The value of \(n_c\) is given as \(n_c \approx 0.8 \times 10^{-1} \, G \, V^{-1}\). Now include (3.109) into the above equation.

\[
\Pi(q^2) = -\frac{4m^2 n_c}{m^2} \left[ \int d^4x \, e^{i q \cdot x} \phi^2(x) x^2 \right] \int d^4y \, e^{i q \cdot y} \phi^2(y) y^2
\]

\[
= -\frac{4m^2 n_c}{m^2} \left[ \int d^4x \, e^{i q \cdot x} \phi^2(x) x^2 \right]^2
\]

(3.112)

Taking (3.96) into account, we have

\[
\int d^4x \, e^{i q \cdot x} \phi^2(x) x^2 = \frac{\rho_c^2}{\pi^2} \int d^4x \, e^{i q \cdot x} / [x^2 + \rho_c^2]^3
\]

(3.113)

Using the \(D\)-dimension identity [26].

\[
d^Dk = k^{D-1} dk d\omega = \frac{2\pi^{\lambda-1}}{\Gamma(\lambda + 1)} k^{2\lambda-1} dk
dk
\]

(3.114)

which for our \(D \equiv 4\) case is.

\[
d^4k = 2\pi^2 x^3 dx d\hat{x}
\]

(3.115)

With this result, we have

\[
\int d^4x \, e^{i q \cdot x} \phi^2(x) x^2 = 2\rho_c^2 \int dx \, d\hat{x} \, x^3 e^{i q \cdot x} / [x^2 + \rho_c^2]^3
\]

(3.116)
Utilizing the following results [26],

\[
\int d^2 x e^{i q \cdot x} = 2 J_1(\sqrt{x^2 q^2})/\sqrt{x^2 q^2}
\]  \hspace{1cm} (3.117)

and using the following identity [110],

\[
\int_0^\infty dx J_1(bx)x^2/[x^2 + a^2] = \frac{a^{-1}b^2}{8} K_{-1}(ab)
\]  \hspace{1cm} (3.118)

where \( J_1 \) is the first order Bessel function and \( K_{-1} \) is the modified Bessel function.

\[
\int d^4x e^{i q \cdot x} \phi^2(x) x^2 = \frac{4 \rho_i^2}{|q|^2} \int_0^\infty dx \frac{x^2 J_1(\sqrt{x^2 q^2})}{x^2 + \rho_i^2} dx
\]
\[
= \frac{4 \rho_i^2 q^2}{|q|^2} \frac{1}{\rho_i 8} K_{-1}(q \rho_i)
\]  \hspace{1cm} (3.119)

Inserting these results back to (3.112), we obtain the single instanton contribution to the spin one scalar channel’s correlation function.

\[
\Pi(q^2) = - \frac{4m_n^2}{m_e^2} \frac{1}{4} \rho_e q^2 [K_{-1}(q \rho_e)]^2
\]
\[
= - \frac{m_n^2}{m_e^2} \rho_e q^2 [K_{-1}(q \rho_e)]^2
\]  \hspace{1cm} (3.120)

Now we want to calculate the instanton contribution to the Laplace sum rule \( R_0(\tau) \).

\[
R_0(\tau) = \frac{1}{\pi} \int_0^\infty dt \text{Im}(t)e^{-\tau t}
\]  \hspace{1cm} (3.121)

As we discussed previously, for all practical QCD calculations, work is always done in the Euclidean domain \( (Q^2 = -q^2) \) away from positive real \( q^2 \) axis. In the Euclidean domain, \( Q^2 = te^{\pm \pi} \) above and below the real \( q^2 \) axis respectively.
Using the following identities \[111\].

\[ K_1(z) = \frac{1}{2} \pi i e^{\pi z} H_1^{(1)}(z) e^{\frac{1}{2} \pi z} \quad (-\pi < \text{arg}(z) \leq \frac{\pi}{2}) \] (3.122)

\[ K_1(z) = \frac{-1}{2} \pi i e^{-\pi z} H_1^{(2)}(z) e^{\frac{1}{2} \pi z} \quad \left( -\frac{\pi}{2} < \text{arg}(z) \leq \pi \right) \] (3.123)

where the \( H_1^{(1)} \) and \( H_1^{(2)} \) are first order Hankel functions.

\[ H_1^{(1)} = J_1 + i Y_1, \quad H_1^{(2)} = J_1 - i Y_1 \] (3.124)

where \( Y_1 \) is the first order Weber function (Bessel function). Notice that \( K_{-1} = K_1 \) and \( \sqrt{Q^2 \rho_c^2} = \sqrt{e^{\pi z} \rho_c} \), so that \( \Pi(t) \) above the real \( q^2 \) axis takes the form.

\[ \Pi(t + i\epsilon) \sim -t \left[ -\frac{\pi}{2} H_1^{(2)}(\sqrt{t \rho_c}) \right]^2 \] (3.125)

Below the real \( q^2 \) axis, \( \Pi(t) \) takes the form as

\[ \Pi(t - i\epsilon) \sim -t \left[ -\frac{\pi}{2} H_1^{(1)}(\sqrt{t \rho_c}) \right]^2 \] (3.126)

Subtracting the above two equations and taking the imaginary part.

\[ \text{Im} \Pi^{\text{int}}(t) = \frac{[\Pi(t + i\epsilon) - \Pi(t - i\epsilon)]}{2i} \]

\[ = -\pi^2 \frac{m^2 c_0^2 \rho_c^2}{2m^2} t Y_1(\sqrt{t \rho_c}) J_1(\sqrt{t \rho_c}) \] (3.127)

Inserting the expression for \( \text{Im} \Pi(t) \) back into \( R_0 \), we have the instanton con-
tribution to the Laplace sum rule \( R_0(\tau, s_0) \) [112]

\[
R_0(\tau) = -\int_0^{s_0} \frac{m^2 n_c \rho^2_c}{2m_c^2} t Y_1(\sqrt{t} \rho_c) J_1(\sqrt{t} \rho_c) e^{-\tau t} \, dt \tag{3.128}
\]

The effective quark mass \( m_* \) acquired in the instanton vacuum is [76, 38]

\[
m_* \approx \frac{2}{3} \pi^2 \langle qq \rangle \rho^2_c \tag{3.129}
\]

in conjunction with the relation \( \langle qq \rangle = -\frac{2\pi}{m_*} \) between the instanton density and the quark condensate [34, 108]. We obtain the following relation.

\[
\frac{\mu \rho^2 \pi}{2m_c^2} = \frac{3}{8\pi} \tag{3.130}
\]

Inserting this relation back to (3.128), we obtain the final form of the \( I = 0 \) channel instanton contribution to the Laplace sum-rule \( R_0 \).

\[
R_0(\tau, s_0)_{I=0} = -\int_0^{s_0} \frac{3m^2(\tau)}{8\pi} t Y_1(\sqrt{t} \rho_c) J_1(\sqrt{t} \rho_c) e^{-\tau t} \, dt \tag{3.131}
\]

where the light quark mass \( m(\tau) \) denotes the running mass (function of \( \tau \)).

The \( I = 1 \) channel’s single-instanton contribution has the same magnitude but with an opposite sign.

\[
R_0(\tau, s_0)_{I=1} = \int_0^{s_0} \frac{3m^2(\tau)}{8\pi} t Y_1(\sqrt{t} \rho_c) J_1(\sqrt{t} \rho_c) e^{-\tau t} \, dt \tag{3.132}
\]

It is worth noting that they are the unique instanton correlation results we obtained [112, 113].

Prior to our research, the single instanton effects employed in the literature
took the following form (in the $I = 0$ channel as an example) \cite{76, 108, 114}.

\[ R_{0}^{\text{inst}}(\tau, s_0) = \frac{3p^2m^2(\mu)}{16\pi^2r^2} e^{-\rho^2/2\pi} \left[ K_0 \left( \frac{\rho^2}{2\pi} \right) + K_1 \left( \frac{\rho^2}{2\pi} \right) \right] \]

(3.133)

where $K_0$ and $K_1$ are the zero order and the first order Modified Bessel functions. This form of instanton effects (3.133) on the correlation function can be understood as an integration, resulting in the following expression \cite{76, 108, 114}.

\[ R_{0}^{\text{inst}}(\tau, s_0) = \frac{1}{\pi} \int_{0}^{\infty} \text{Im} \Pi^{\text{inst}}(\tau) e^{-\tau t} d\tau \]

(3.134)

where the $\Pi^{\text{inst}}(\tau)$ has the same expression as in (3.127). We can verify the conclusion by using the identity \cite{110}.

\[-\pi \int_{0}^{\infty} J_0(x)Y_0 e^{-x^2} x^2 dx = \frac{1}{2\pi} e^{-1} \int_{-\infty}^{\infty} K_0 \left( \frac{1}{2s} \right) \]

\[ H_0(s) = \frac{1}{(2s)^3} e^{-1/2s} \left[ K_0 \left( \frac{1}{2s} \right) + k_1 \left( \frac{1}{2s} \right) \right] \]

(3.135)

Taking the asymptotic limits in Eq. (3.131) ($s_0 \to \infty$), we find that our result (3.131) is equivalent to the widely used one (3.133). The only difference between these two expressions is the integral ranges used: the integral range is from 0 to $\infty$ in (3.131) and the range is from 0 to $s_0$ in (3.133). We will discuss these two results in Chapter 4 and conclude that our result is the correct understanding of single-instanton effects in the continuum contributions.
3.4 Hadronic Models

In this thesis, we employ the Laplace sum rule $R_0$ to investigate the lowest-lying resonance's properties such as the corresponding continuum onset $s_0$, the mass $M$ and decay-width $\Gamma$ in the $I = 0, 1$ scalar channels.

$$R_0 = \frac{1}{\pi} \int_0^\infty \text{Im} \Pi(t) e^{-it} dt$$  (3.136)

After the field-theory content of $\text{Im} \Pi(t)$ has been inserted in the above equation, this expression can be related to some hadronic model, i.e. the hadronic spectral function. In this way, our theoretical results can be related to experimental data, which in turn gives our QCD sum rules prediction power.

The narrow resonance approximation has been widely used in the literature following the seminal work of SVZ [34]. In that paper, the spectral ansatz is described as a delta function plus a continuum theta function.

$$\rho(s) = a \delta(s - M^2) + \theta(s - s_0) \text{Im} \Pi^{QCD}(s)$$  (3.137)

where $a$ are some constants. The delta function denotes the contribution of the lowest-lying resonance and the theta function the contribution from above the continuum onset $s_0$. By implementing this ansatz, the narrow width approximated subcontinuum resonances contribute to the light-quark (linear combination of $u$ and $d$ quarks) two-point correlation function as a sum of delta functions.

$$\text{Im} \Pi(s)_{res} = \text{Im} \sum_r \left[ \frac{g_r}{(s - m_r^2) + im_r \Gamma_r} \right]$$

$$= \sum_r \left[ \frac{g_r m_r \Gamma_r}{(s - m_r^2)^2 + m_r^2 \Gamma_r^2} \right] \rightarrow \sum_r \pi g_r \delta(s - m_r^2)$$

(3.138)
The coupling coefficient \( g_r \) is proportional to \( m_r^2 \). However, the constant of proportionality is expected to be much larger for \( \bar{q}q \) resonances, \textit{i.e.} resonances that coupling directly to the field-theoretical operators in the scalar current (1.33), than for exotic resonances [115]. It is for precisely this reason that sum-rule searches for non-\( \bar{q}q \) scalar resonance states, such as \( \bar{K}K \) molecules [84] or glueballs [79], utilize correlation functions based on appropriate \( \bar{K}K \) or gluonic currents that coupling directly to such hadronic exotica.

Inserting the above spectral ansatz back into (3.136), the narrow approximation hadronic model content of Laplace sum rules can be obtained.

\[
R_0(\tau) = \sum g_r e^{-m_r^2 \tau} \quad (3.139)
\]

where \( R_0(\tau) \) contains the theoretical content of the sum-rule. Note in the above narrow width approximation approach, we implicitly assume the anticipated local duality between QCD and hadronic physics above some appropriately chosen continuum threshold \( s > s_0 \) [57, 58]. As discussed in previous chapters, the condensates and instanton contributions to \( \Pi(q^2) \) are non-perturbative effects which implies the momentum involved is small in the region dominated by these effects. With properly chosen \( s_0 \) (in almost all QCD sum rules applications \( s_0 \) is sufficient higher than \( 1 \mathrm{GeV}^2 \)), all field-theory contents above \( s_0 \) are nearly purely perturbative. The continuum contribution also represents the effective summation over excitations which are too weak to be directly observed.

Despite its relative success, especially in the calculation of low-resonance properties of vector and axial-vector channels, the narrow-resonance approximation is insufficient in dealing with broad lowest-lying resonances because it totally ignores the width effects of the resonances. For example, the \( \sigma \) meson
as quoted from [50] has a width from 400 to 1200 MeV. Without finite width effects, QCD sum rules provide incomplete results for the $I = 0, 1$ channels. Thus the narrow-resonance approximation requires significant modification to fit the requirements of this research.

For Laplace sum rules, a more quantitative estimate of resonance-width effects could be a replacement of the delta function in (3.139), which should be understood as the narrow-width limit of the Breit-Wigner shape, by the Breit-Wigner peak [50], and then substituting into the Laplace sum-rule definition (3.34).

\[
\pi g_r \delta(s - m_r^2) = \lim_{\Gamma_r \to 0} \frac{1}{(s - m_r^2 + i m_r \Gamma_r)}
\]  

(3.140)

However, the Breit-Wigner shape has an infinite tail, and significant portions of that tail may extend above the continuum threshold $s_0$ or below the $s = 0$ boundary into Euclidean momenta as shown in Figure 3.7.
Figure 3.7: Breit-Wigner shape of resonance width. This Breit-Wigner peak is centered at $M = 1 \text{GeV}$ and with a $200 \text{MeV}$ width effect. Assuming a continuum threshold occur at $s_0 = 2 \text{GeV}^2$, the shaded area of the Breit-Wigner tails ($s > s_0$ and $s < 0$) are truncated in QCD sum rule calculations.
Such contributions from the Breit-Wigner tail, whether included or truncated away, can be substantial for resonances with widths in excess of 100 MeV [113], and can be a source of theoretical uncertainty in Laplace sum-rules analysis of broad sub-continuum resonances.

This uncertainty may be understood as a limitation on the Laplace sum-rule methodology itself, particularly for channels in which the lowest-resonance is broad or more than one resonance lies below the continuum threshold. Non-lowest-lying resonances are expected to be less stable, and consequently, to be substantially broader than lowest-lying resonances in most channels. For example, the $I = 1$ pseudoscalar channel has a narrow lowest-lying resonance $\Pi$ and a substantial broader excitation state resonance $\Pi(1300)$ with a width as large as 600 MeV [50]. For this channel, a modified Breit-Wigner width effect beyond narrow approximation has been employed with relatively convincing results [113, 116].

Probably an even more important reason to prevent us from employing Breit-Wigner form of width-effects, is a computational obstacle. If the Breit-Wigner shape is used directly, the following integration occurs in the $R_0$ sum-rule calculation.

$$\int_0^{\infty} I m \left( \frac{-1}{t - M^2 + iM\Gamma} \right) e^{-t\tau} dt$$

$$\Rightarrow \int_0^{\infty} \left( \frac{M\Gamma}{(t - M^2)^2 + M^2\Gamma^2} \right) e^{-t\tau} dt \quad (3.141)$$

This integration doesn’t have a simple form solution, and we have to employ this integration’s result as an intermediate stage in the least-$\chi^2$ simulation (to be discussed later). Therefore, the complicated form of the Breit-Wigner shape integral solution makes our tasks difficult within any reasonable computation time given available computing power.
In summary, to overcome the computational difficulties of Breit-Wigner shape in the simulation program and the possibly large portion of the infinite Breit-Wigner tail above the Laplace sum-rule energy release region, a simplified modification of Breit-Wigner shape is needed.

Instead of the delta function, the Breit-Wigner shape on the right-hand side of above equation (3.140) can be expressed as a Riemann sum of unit area pulses \( P_m \), centered at \( s = m^2 \) [117].

\[
P_M[i\,s, \Gamma] = \frac{1}{2\,\Gamma}\left[\Theta(s - M^2 + M\Gamma) - \Theta(s - M^2 - M\Gamma)\right]
\]  \hspace{1cm} (3.142)

\[
I_m = \frac{-1}{2\,\Gamma^2 + (s - M^2)^2} = \frac{M\Gamma}{(s - M^2)^2 + M^2\Gamma^2}
\]

\[
= \lim_{n \to \infty} \frac{1}{n} \sum_{j=1}^{n} \sqrt{\frac{n - j + f}{j - f}} P_M \left[ s, \sqrt{\frac{n - j + f}{j - f}\Gamma} \right]
\]  \hspace{1cm} (3.143)

where \( f \) is any arbitrarily chosen constant between 0 and 1. If one approximates the resonance shape via (3.143) by truncating \( n \) to some finite number of pulses, then the approximation (unlike the \( n \to \infty \) limit) becomes sensitive to the choice of \( f \). The value for \( f \) may be chosen to ensure that the area under the truncated sum is equal to the area under the true resonance shape.

\[
\int_{-\infty}^{\infty} \frac{M\Gamma}{(s - M^2)^2 + M^2\Gamma^2} ds = \pi
\]  \hspace{1cm} (3.144)

In this thesis, \( n = 4 \) is picked. Putting \( n = 4 \) back to the above equation, we obtain an area of \( \pi \) by choosing \( f = 0.70 \). An example of the four-pulse approximation is chosen in Figure 3.8.

The accuracy of the finite-width approximation scheme depends on the number of the square-pulses employed. On the one hand, if the approximation
has too few pulses, for example only one or two pulses, the Breit-Wigner shape
would not be represented accurately, and the final simulation results will over-
estimate the true width effects. On the other hand, if the approximation has
too many pulses (for example 6 square-pulses approximation). and when the
resonance width is large than 200 MeV, the widest pulses may extend below
$s = 0$ or above the continuum threshold $s_0$ boundary in physical domain, which
is what we try to avoid. Therefore, in the scalar meson cases (where width
effects could be larger than 200 MeV), the four square-pulse approximation is
a suitable choice.

Compared with the narrow-resonance approximation (3.139), we find the
non-zero width $\Gamma_r$ for the corresponding subcontinuum resonance modifies the
hadronic content of $R_0$.

\[ R_0(\tau) = \sum_r g_r W(M_r, \Gamma_r, \tau) e^{-M_r^2\tau} \]  \hspace{1cm} (3.145)

In the four pulse approximation, the width-effect function $W(M, \Gamma, \tau)$ reads
as.

\[ W[M, \Gamma, \tau] = 0.5589 \Delta(M, 3.5119\Gamma, \tau) - 0.2294 \Delta(M, 1.4412\Gamma, \tau) \]
\[ -0.1368 \Delta(M, 0.8597\Gamma, \tau) - 0.0733 \Delta(M, 0.4606\Gamma, \tau) \]  \hspace{1cm} (3.146)

The $\Delta$ function can be derived as.

\[ e^{-M^2\tau} \Delta(M, \Gamma, \tau) = \int_{-\infty}^{\infty} P_M(s, \tau) e^{-s\tau} ds \]
\[ = \int_{-\infty}^{\infty} \frac{1}{2M\Gamma} \left[ \Theta(s - M^2 + \Gamma) - \Theta(s - M^2 - \Gamma) \right] e^{-s\tau} ds \]
\[ = \frac{1}{2M\Gamma} (e^{M\Gamma\tau} - e^{-M\Gamma\tau}) e^{-M^2\tau} \]  \hspace{1cm} (3.147)
Figure 3.8: An example of the 4 square-pulse approximation to the Breit-Wigner resonance shape obtained by truncating equation(3.143) to $n = 4$, and by choosing $f = 0.701$ to ensure that the area under the four pulses is equivalent to the total area under the Breit-Wigner curve. This particular example is for a mass $M = 680\, \text{MeV}$ and width $\Gamma = 100\, \text{MeV}$.
\[ \Delta(M, \Gamma, \tau) = \frac{\sinh(M\Gamma\tau)}{M\Gamma\tau} \]  

(3.148)

We can check explicitly that when \( \Gamma \) approaches to zero the width effect because \( W(M, \Gamma, \tau) \to 1 \) as expected.

Now equating the theoretical contents with the wide-effect hadronic ansatz, we obtain the final equation we will employed in the \( I = 0, 1 \) mesons study.

\[ R_{0|j}^{\text{pert}} + R_{0|j}^{\text{cond}} + R_{0|j}^{\text{inst}} = \sum_{r} g_{r} W_{r|j} M_{r|j} \Gamma_{r|j} \tau e^{-M_{r|j}^{2} \tau} \]  

(3.149)

where \( g_{r} \) is the strong coupling coefficient.

Now let us investigate the right-hand side of the above equation, i.e. the hadronic content of Laplace sum rules. Laplace sum rules are used here since they enhance the lowest-lying resonance's contribution and suppress the continuum contribution. If the higher-mass resonance's mass is around the continuum onset \( s_{0} (M_{r}^{2} \sim s_{0}) \), it will be absorbed in the continuum part. If its mass is substantial below \( s_{0} \), the higher-mass subcontinuum resonance will be exponentially suppressed due to the \( e^{-M_{r}^{2} \tau} \) term in the integration. Thus, it is safe to conclude that Laplace sum rules are most sensitive to the low-lying resonances [34, 41].

In this thesis, we look at the possibility of more than one resonance hadronic models and find only one subcontinuum finite-width resonance model is reasonable in the \( I = 0, 1 \) scalar channels (Detailed analysis will be provided in the next chapter). For now, the spectral model is still written as a sum of \( r \) subcontinuum resonances.

To summarize, the field-theoretical contribution from QCD to the fundamental Laplace sum-rule \( R_{0|j}(\tau, s_{0}) \) is related to the phenomenological model
through the following equation.

\[ [R_0(\tau, s_0)]_{/f=0.1} = \sum_r a_r W[M_r, \Gamma_r, \tau] e^{-M_r \tau} \]  
(3.150)

The field-theory content of the QCD sum rules is.

\[ [R_0(\tau, s_0)]_{/f=0.1} = [R_0(\tau, s_0)]^{pert} + [R_0(\tau)]^{cond} + [R_0(\tau, s_0)]^{inst}_{/f=0.1} \]  
(3.151)

where \([R_0(\tau, s_0)]^{pert}\), \([R_0(\tau)]^{cond}\) and \([R_0(\tau, s_0)]^{inst}_{/f=0.1}\) are given in (3.44), (3.87), (3.131) and (3.132).

\[ R_0^{cond}(\tau) = m^2 \left[ \frac{3}{2} < mqq > + \frac{1}{16\pi} < \alpha_s G^2 > - \frac{88 \pi \tau}{27} < \alpha_s(qq)^2 > \right] \]  
(3.152)

\[ R^{inst}(\tau)_{/f=0.1} = \frac{3m^2}{8\pi} \int_0^{s_0} s e^{-\tau s} Y_1(\rho \sqrt{s}) J_1(\rho \sqrt{s}) \, ds \]  
(3.153)

\[ R_0^{pert}(\tau) = \frac{3m^2}{16\pi^2 \tau^2} \left( 1 + \frac{17}{3} \frac{\alpha}{\pi} \right) \left[ 1 + s_0 \tau \right] e^{-s_0 \tau} \]  
(3.154)

\[ - 2 \frac{\alpha}{\pi} \left[ 1 - \gamma_E - e^{-s_0 \tau} - E_1(s_0 \tau) - (1 - s_0 \tau) e^{-s_0 \tau} \log(s_0 \tau) \right]. \]
Chapter 4

QCD Sum-Rule Analysis

4.1 Rationale of Our Approach of QCD Sum-Rule Analysis

4.1.1 Possible Problems of Traditional Approaches

Having given the relation between QCD field theoretical contents and the spectral model via dispersion relations, the next task is the QCD sum-rule analysis to extract the properties of certain hadrons in the channel with corresponding quantum numbers.

The underlying principle of field theoretical approaches to hadronic phenomenology is the duality assumption. That is, it is possible to simultaneously describe a hadron as quarks propagating in the QCD vacuum, and as a phenomenological field with the appropriate quantum numbers. The duality matching must be done consistently and systemically in order to make the results obtained from QCD sum-rules acceptable under scrutiny. Unfortunately, typical QCD sum-rule analyses of hadron properties in the literature fall short in the following ways [118].

1. Selecting a single value for the Borel parameter ($\tau$) which give “nice” results. A Borel regime (i.e. $\tau$ range) should be selected to meet the stability and reliability requirements in QCD sum-rule analysis.

2. Selection of the Borel regime without careful regard to the balance of the OPE contributions and the continuum contributions (the contributions from above the $s_0$ threshold), which can be approximated by purely
perturbative calculation.

3. Fixing of parameters (such as the continuum threshold $s_0$) to preferred values. It becomes apparent that this introduces a strong bias to the remaining fit parameters, which may not reflect the properties of QCD correctly.

4. Claiming an accuracy for QCD sum-rule predictions without supporting calculations. Occasionally a "stability analysis" [119, 120] is considered, in which fit parameters are monitored as single independent variables whose value is varied once at a time. However, such analyses explore a relatively small corner of the parameter space.

In this research, we try to design a more rigorous approach to extract the hadronic parameters from the field theory content of the Laplace sum-rule.

### 4.1.2 Traditional Ratio Method

One of the common methods is the derivative sum-rule and ratio method originated from SVZ [34]. The basic idea is that it is possible to isolate the meson's mass of interest as a function of the Borel scale $\tau$, by taking a ratio of the first derivative sum-rule $R_1(\tau, s_0)$ with the fundamental sum-rule $R_0(\tau, s_0)$. As we discussed before, the first derivative sum-rule is defined as,

$$ R_1(\tau, s_0) = \frac{1}{\pi} \int_0^{s_0} \text{Im}(\Pi(s)) e^{-\tau s} ds $$

This approach has some aesthetic appeal and has widely become the method of choice for analyzing QCD sum-rules. The continuum threshold $s_0$ is selected to make the ratio of the two sum rules $R_1(\tau, s_0)/R_0(\tau, s_0)$ as flat a function of $\tau$ as possible. Finally, the meson's mass is selected from the point at which the ratio is most flat or stable. Unfortunately, this method has some shortcomings:
1. Inherently, this method carries an ambiguous feature. The $s_0$ is determined by "as flat as possible" and the mass by "as most flat". These criteria imply there is no quantitative, mathematical determination scheme. The extraction of information from the sum-rule is judged by human feelings but not a rigorous method independent of human interference.

2. The ratio method does not check the validity of each individual sum rule. It is possible to have individual sum rule that is not valid while their ratio is a flat function of $\tau$ [118]. In addition, the ratio method can not account for the fact that sum rules do not work equally well. The Borel regime where a sum rule is valid can vary from one sum rule to another. Moreover, large uncertainties in one sum rule can spoil the predictions of another sum rule. For example, in reference [121] a detailed comparison of fundamental ($R_0$) and derivative ($R_1$) sum rules is carried out for the $\rho$ meson (i.e. the vector channel), and found the valid Borel regime for the derivative sum rule shrink nearly to non-existent but the ratio still gives a flat bottom.

In practice, the predictions based on the fundamental sum rule are more reliable than those from the derivative sum rules $R_n$. As $n$ increases in the derivative sum rules $R_n$, the perturbative contribution of $R_n$ becomes more dependent on the continuum threshold $s_0$ (remember Laplace sum rules are designed to be relatively insensitive to $s_0$), and the condensate contribution of $R_n$ becomes more dependent on the higher dimensional condensates' contributions, which are not as well estimated as lower dimensional condensates' contributions. Therefore, we conclude that $R_n$ becomes less and less reliable as $n$ increases [116, 118]. Moreover, there is no guarantee the $s_0$ is universal for all $n$. 

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Based on the above argument, we employ the fundamental sum-rule $R_0(s_0, \tau)$ as the theoretical prediction tool rather than the ratio method discussed above. The utilization of $R_0(\tau, s_0)$ to extract information from the QCD field-theoretical calculation is the content of next section.

4.1.3 Our Approach of QCD Sum-rule Analysis

In this thesis, a method of quantitatively determining of phenomenological quantities with and without an uncertainties estimate will be presented. The following is the outline of our approach:

1. Utilizing the Hölder inequality technique to determine the appropriate Borel regime ($\tau$) for QCD sum-rule analysis in the channels of interest.

2. Developing a least-$\chi^2$ approach in a multiple parameter set to extract the desired information from the QCD sum-rule.

3. Selecting the optimization algorithm to determine the least $\chi^2$ within the $\tau$ range determined from the above step.

4. Extracting the optimization values of the spectral ansatz’s parameters by minimizing the $\chi^2$ value (Best-fit approach).

5. Estimating uncertainties associated with the corresponding channels' QCD sum-rule.

The first step will help us to obtain a rigorous quantitative region in which the continuum and OPE contribution will be balanced so as not to destroy the stability of the QCD sum-rule. From the Hölder estimation, we hope the first two possible problems in the traditional analyses can be avoided. In the second step, we use the least-$\chi^2$ method to get rid of the vague nature of the traditional QCD ratio methods [34] (will be discussed later). In the final
step, all sources of uncertainties associated with scalar channels are taken into account simultaneously to search the stability and accuracy of the analysis results.
4.2 Least-$\chi^2$ Methods

4.2.1 Estimate of QCD Sum-rule Inputs

In the QCD sum-rule equation (3.150), several inputs are needed to conduct the sum-rule analysis. Since the RG invariant mass $m$ is absorbed in the right-hand side of (3.150), the values of the needed input parameters for this QCD sum-rule are the QCD scale $\Lambda$, the quark condensate $\langle \bar{q}q \rangle$, the gluon condensate $\langle \alpha GG \rangle$, the vacuum saturation factor $f_{ss}$, the dimension six condensate $\langle a\bar{q}q\bar{q}q \rangle$ and the instanton size $\rho_i$. In assigning the standard values and the uncertainties for these parameters, we follow two general principles:

1. we would like to select the standard values in according with the generally accepted values in the literature.

2. we would like to select the uncertainties conservatively enough such that the QCD sum-rule approach can test the validity of our present understanding of QCD and at the same time, we would like to cover as much as possible the different parameters' values argued and employed in the literature.

Now we discuss these standard values and their uncertainties respectively.

- The QCD scale $\Lambda$ (normalization point) is dependent on the renormalization scheme employed. It is generally found that the QCD sum-rule analysis is insensitive to a change in $\Lambda$ [42, 34]. Throughout this thesis, we choose the three-flavour $\overline{MS}$ scheme value $\Lambda = 300$ MeV [33, 50].

- For the quark condensate $\langle m\bar{q}q \rangle$, we use the standard value in most of the QCD sum-rule analysis obtained from PCAC Gell-Mann-Okubo relation [122], $\langle m\bar{q}q \rangle = -f^2_\pi m_\pi^2/2$ with the physical values of $m_\pi = 140$ MeV and
$f_\pi = 93 \text{ MeV}$. If we assume $m_u + m_d = 11 \text{ MeV}$, this implies the standard value $\langle \bar{q}q \rangle = -250 \text{ MeV}^{-3}$. However, QCD sum-rule considerations of octet baryon magnetic moments [123] prefer a smaller magnitude at $\langle \bar{q}q \rangle = -225 \text{ MeV}^{-3}$ which is about 10% smaller than the standard value we used.

- The gluon condensate $\langle \alpha G G \rangle$ estimated from charmonium sum rules [34] has become the standard value for Borel sum rules $\langle \alpha_s \xi G G \rangle = 0.014 \text{ GeV}^{-1}$ with a variation about 30% [118, 124].

- Relatively little is known about the magnitude of the dimension-six, four-quark condensate. Its value is obtained by employing the so-called vacuum saturation hypothesis $\langle \bar{q}qqq \rangle = f_{rs} \langle \bar{q}q \rangle^2$, where the $f_{rs}$ is the vacuum saturation factor. Early arguments placed the value of this condensate within 10% of the factorized values [106], where $f_{rs} = 1$. However, other analyses claimed significant violation of factorization for these four-quark operators in both meson and nucleon sum rules [120, 124, 125, 126]. In references [124, 127], the authors claimed the violation is as large as a factor of 2. Therefore, in this work, we choose the average value $f_{rs} = 1.5$ with a variation range $1 < f_{rs} < 2$.

- The single instanton size $\rho_c$ used in this research follows the classical paper of Shuryak [67] and SVZ [34] where $\rho_c = 1/(600 \text{ MeV})$. This number has been accepted as a standard value for single-instanton effects in most of the QCD sum-rule analysis. In SVZ's paper, the authors concluded that it is completely unreasonable to speak about an instanton with dimension exceeding $1/500 \text{ MeV}$. Thus we give a 15% variation space for the instanton size.
4.2.2 Hölder Inequality

The first thing needed for this QCD sum-rule analysis is the determination of the valid $\tau$ ranges for both $I = 0, 1$ channels. The determination of a valid $\tau$ range in a given channel has always been a source of uncertainty in QCD sum rule analyses even since its innovation [34]. In that paper, SVZ argued [34]:

1. The sum rule are expected to be valid as long as the power corrections (the higher dimension condensate terms) do not dominate, and $\tau$ is bounded from below that point.

2. The low $\tau$ boundary is determined such that the integral over the cross section is dominated by a single resonance and the continuum contributions are not too large.

Following the above two statements, SVZ roughly estimated a valid $\tau$ range for the $\rho$ meson application. From then on, most of the QCD sum rule applications determine the $\tau$ range without systematical and rigorous methods. In conclusion, the determination of the $\tau$ regime in the literature always falls into the following two categories:

1. The determination method has no quantitative analysis. The $\tau$ range is just roughly estimated such as the SVZ case.

2. The determination method has some quantitative analysis, but the criterion utilized lack of solid ground. One example is presented in [118]. In that paper, the $\tau$ range is chosen such that the highest dimension operator(s) contribute no more than 10% to the QCD side while the continuum contribution is less than about 50% of the total phenomenological side. The former sets a criterion for the convergence of the OPE (i.e. the high $\tau$ boundary) while the latter controls the continuum contribution (i.e. 
the low \( r \) boundary). However, the selection of 10\% and 30\% is kind of arbitrary and lack a solid theoretical argument.

In order to avoid the above controversy in determining \( r \) regime, we employ a new technique. the QCD sum-rule inequalities method developed in [128]. This new technique is based on the Hölder integral inequality, which provides fundamental constraints on QCD sum rules. These constraints must be satisfied if the QCD sum rules are to consistently describe integrated physical cross-sections, which are related to the integration of imaginary part of two-point correlation functions. An important feature of the inequality method is that these constraints do not require any phenomenological input (such as the 10\% of higher-dimension OPE contribution and the 50\% of the continuum contribution as stated in Leinweber’s work). Therefore it provides universal quantitative constraints on any QCD sum rules.

Using this technique, non-trivial information constraining the continuum threshold \( s_0 \) and sum-rule energy scale \( r \) will be obtained. This information then provides insight into the issues concerning the continuum hypothesis and the energy range in which the sum-rules are reliable. To our purpose here, our main concern is to obtain the \( r \) range suitable for our Laplace sum rules. Then we use the continuum threshold \( s_0 \) obtained from QCD sum-rule analysis to compare with inequality’s provided \( s_0 \) as a consistency check.

Hölder’s inequality for integrals defined over a measure \( d\mu \) is [129, 130].

\[
\left| \int_{t_1}^{t_2} f(t)g(t)d\mu \right| \leq \left( \int_{t_1}^{t_2} |f(t)|^p d\mu \right)^{1/p} \left( \int_{t_1}^{t_2} |g(t)|^q d\mu \right)^{1/q}
\]  

(4.2)

where \( \frac{1}{p} + \frac{1}{q} = 1 \) and \( p, q \geq 1 \). When \( p=q=2 \) the Hölder inequality reduces to the well-known Schwarz inequality. The key idea in applying Hölder’s inequality to sum rules is recognizing that for a typical correlation function \( \Pi(q^2) \), \( Im \Pi(q^2) \)
is positive because of its relation to physical cross-sections and can thus serve as the measure \( d\mu = Im\Pi(t) dt \) in (4.2).

Returning to (4.2) with \( d\mu = Im\Pi(t) dt \), the Laplace sum rule \( R_0 \) is defined as in (1.52). Set

\[
f(t) = e^{-at}, \quad g(t) = e^{-bt}
\]

where \( a + b = 1 \) and \( t_1 = 0 \), \( t_2 = s_0 \), we find

\[
\left| \int_{t_1}^{t_2} f(t)g(t)d\mu \right| = \int_0^{s_0} e^{-t\tau}Im\Pi(t) dt = R_0(\tau, s_0)
\]  

(4.4)

\[
\left( \int_{t_1}^{t_2} |f(t)|^p d\mu \right)^{1/p} = \left( \int_0^{s_0} e^{-at\tau}Im\Pi(t) dt \right)^{1/p} = \left[ R_0(ap\tau, s_0) \right]^{1/p}
\]

(4.5)

\[
\left( \int_{t_1}^{t_2} |g(t)|^q d\mu \right)^{1/q} = \left( \int_0^{s_0} e^{-bt\tau}Im\Pi(t) dt \right)^{1/q} = \left[ R_0(bq\tau, s_0) \right]^{1/q}
\]

(4.6)

Put (4.1), (4.5) and (4.6) back to (4.2). we obtain the \( R_0 \) Hölder inequality relation.

\[
R_0(\tau, s_0) \leq R_0^p(ap\tau, s_0) R_0^q(bq\tau, s_0)
\]

(4.7)

In the above equation, if we set \( ap\tau = \tau_{min} \) and \( bq\tau = \tau_{max} \), \( 1/p = \omega \) and \( 1/q = 1 - \omega \), we have

\[
R_0[\omega\tau_{min} + (1 - \omega)\tau_{max}, s_0] \leq R_0[\tau_{min}, s_0] R_0^{1-\omega}[\tau_{max}, s_0]
\]

(4.8)
where \( \tau_{\text{min}} \leq \tau_{\text{max}} \). To analyze the inequality (4.8), we use
\[
\tau_{\text{max}} - \tau_{\text{min}} = \delta \tau = 0.1 GeV^{-2}
\]
to perform a local analysis [131]. The inequality is insensitive to the value of \( \delta \tau \) provided that \( \delta \tau \) is reasonably small (in QCD \( \delta \tau \sim 0.1 GeV^{-2} \) appears sufficient).

The results of this inequality analysis for both \( I = 0 \) and \( I = 1 \) channels are illustrated in Figure (4.1) and (4.2), corresponding to specific values of the condensates and the vacuum saturation factor \( f_{\text{vs}} \) used in the program. In each figure the shaded region represents the admissible \((s_0, \tau)\) parameters space where the Hölder inequality is satisfied.

Referring to the literature [128, 131], there are always two common features that persist in an inequality analysis of valid QCD sum rules:

1. The existence of a lower bound on the continuum threshold \( s_0 \).

2. The existence of an upper bound on the sum rule energy parameter \( \tau \).

This can be viewed as a test of both the validity of the continuum hypothesis \( (i.e. \) the duality hypothesis above continuum threshold \( s_0 \)) and of the upper bound of \( \tau \) (the lowest energy \( \tau = 1/M^2 \), where \( M \) is the Borel parameter).

The second feature gives a constraint on the condensate series. As seen from Figure (4.3), condensate contributions to the QCD sum rule \( R_0(\tau, s_0) \) become more and more important in the high \( \tau \) region, which denotes the truncated higher-dimension condensates and other neglected or unknown effects (such as the vacuum saturation factor) weights in the total sum rule become substantial [34, 118]. In the Hölder inequality analysis, beyond a certain \( \tau \) value in the corresponding channel's \((\tau - s_0)\) space, these condensate effects which are not included in the field content calculation become so large that the integrated property of \( Im\Pi(t) \) is broken. Therefore, the upper bound \( \tau \) parameter indicated a maximal condensate contribution allowed in the QCD sum rule. From Figure
Figure 4.1: The shaded area represents the region in the $s_0 - \tau$ parameter space consistent with the inequality for the light quark $I = 1$ sum-rule (3.150). The input parameter values $f_{us} = 1.5$, $\Lambda = 300 \text{ MeV}$, $\rho = 1/(600 \text{ MeV})$, and $\delta \tau = 0.1 \text{ GeV}^{-2}$ are used in the calculation. The $\tau$ axis is in GeV$^{-2}$ and $s_0$ axis is in GeV$^{-2}$. 
Figure 4.2: The shaded area represents the region in the $s_0 - \tau$ parameter space consistent with the inequality for the light quark $I = 0$ sum-rule (3.150). The input parameter values $f_{\pi\pi} = 1.5$, $\Lambda = 300\,\text{MeV}$, $\rho = 1/(600\,\text{MeV})$, and $\delta\tau = 0.1\,\text{GeV}^{-2}$ are used in the calculation. The $\tau$ axis is in $\text{GeV}^{-2}$ and $s_0$ axis is in $\text{GeV}^{-2}$.
(4.1) and Figure (4.2), we obtain an upper bound of $\tau \sim 1.7 \text{GeV}^{-2}$ in the $I = 0$ channel, and $\sim 1.1 \text{GeV}^{-2}$ in $I = 1$ channel.

The lower bound $\tau$ parameter is obtained by the start point from where a relatively flat bottom ($\tau - s_0$) boundary can be observed. In both $I = 0, 1$ channels, $\tau_{\text{min}} = 0.3 \text{GeV}^{-2}$ is obtained. The low $\tau$ boundary gives a constraint on the continuum contribution (which states above a certain point $s_0$, all contribution to $\int_0^\infty e^{it} \text{Im} \Pi(s) ds$ can be calculated by purely perturbative QCD (i.e. the duality hypothesis). Below the boundary point $\tau_{\text{min}}$, the continuum contribution grows so large that a local variation of $\tau (\delta \tau)$ will violate the inequality constraints on the integration property of $\text{Im} \Pi(t)$, that is the $R_0(\tau, s_0)$ is too sensitive to $s_0$ value below the $\tau_{\text{min}}$. This constraint corresponds to SVZ's conclusion that the one-resonance should dominate the integral over the cross-section and the continuum should not become too strong.

We conclude.

- For the $I = 0$ channel, $0.3 \text{GeV}^{-2} < \tau < 1.7 \text{GeV}^{-2}$.
- For the $I = 1$ channel, $0.3 \text{GeV}^{-2} < \tau < 1.1 \text{GeV}^{-2}$.

4.2.3 Least-$\chi^2$ Approach

In this thesis, a procedure based on an overall fit of the Borel-parameter ($\tau$) dependence of a sum rule's field-theoretical content to the dependence anticipated from resonance properties has been used. This method has drawn wide attention in the community and has been successfully employed in various channels [118]. For example, properties of the first pion-excitation state $\Pi'$ have been obtained by fitting the QCD Borel-parameter dependence for the lowest $\Pi'$-sensitive Laplace sum rule to its corresponding hadronic contents [116, 117]. In this thesis, we obtain a $\chi^2$-minimizing weighted least square fit of $R_0^{I=0.1}(\tau, s_0)$ to the $\tau$-dependence anticipated from the corresponding hadronic
models. In other words, our fit is generated by obtaining values for \( m_r, \Gamma_r, s_0 \) and the resonance's coupling factor \( a_r \) that minimize a least-square fit of QCD field content with properly chosen weighting function,

\[
[R_0(\tau, s_0)]^{f=0.1} = \sum_r a_r W_r(m_r, \Gamma_r, \tau) e^{-m_r^2} \tag{4.9}
\]

where the left-hand side \( R_0(\tau, s_0) \) has the following form.

\[
[R_0(\tau, s_0)]^{f=0.1} = \frac{3m^2}{16\pi^2\tau^2} \left( \left[ 1 + \frac{17}{3}\alpha \right][1 + s_0\tau]e^{-s_0\tau} - \frac{2\alpha}{\pi} \left[ 1 - \gamma_c + e^{-s_0\tau} + E_1(s_0\tau) + (1 + s_0\tau)e^{-s_0\tau}\log(s_0\tau) \right] \right) + \frac{3m^2}{2}(m\bar{q}q) + \frac{1}{16\pi m^2}(\alpha \times GG) - \frac{88m^2}{2\pi} f_{\alpha}(\alpha(\bar{q}q)^2)\tau
\]

\[
= \int_0^{s_0} \frac{3m^2(\tau)\bar{t}_1(\sqrt{t}\rho_c)J_1(\sqrt{t}\rho_c) e^{-t}}{8\pi} dt \tag{4.10}
\]

In our case, we denote the \( \chi^2 \) weighting function as \( \epsilon(\tau, s_0) \). Selecting \( N \) evenly distributed points in the allowed \( \tau \) parameter space (Borel scale region) \( \tau_i, i = 1 \ldots N \), the \( \chi^2 \) is defined as.

\[
\chi^2 = \frac{1}{N} \sum_{n=1}^{N} \left[ [R_0(\tau_n, s_0) - a W_r(m_r, \Gamma_r, \tau) e^{-m_r^2}]^2 / \epsilon(\tau_n, s_0) \right] \tag{4.11}
\]

The selection of weighting function is important in this work. Two criteria guide the selecting of the weighting function \( \epsilon(\tau, s_0) \).

1. The weighting function should reflect the uncertainties associated with Laplace sum rule \( R_0(\tau, s_0) \).

2. The uncertainties in \( R_0(\tau, s_0) \) are not uniformly distributed throughout the Borel regime, therefore, the weighting function should manifest this property as well.
Now we investigate the total uncertainty of sum rule \( R_0(\tau, s_0) \). Let us start from the condensate uncertainties of \( R_0 \). The gross effect comes from the uncertainty of quark condensate, the gluon condensate and the four-quark condensate.

For now, the vacuum saturation hypothesis is assumed as exactly in the four-quark condensate calculation. that is \( \langle \bar{q}q\bar{q}q \rangle = \langle \bar{q}q \rangle^2 \) where \( f_{cs} = 1 \) (the variation of \( f_{cs} \) will be left in the Monte Carlo simulation). The uncertainty of the dimension six condensate comes from the accumulation of the quark condensate \( \langle \bar{q}q \rangle \) uncertainty.

Figure (4.3) is the ratio of total condensate effects over \( R_0 \) in the \( I = 0 \) channel. We find the condensate effects become large on Laplace sum rule only at the high end of \( \tau \) region mainly because the four quark condensate term contribution in (3.150) \( \langle \bar{q}q \rangle^2 \tau \) grows as \( \tau \) increases.

We can conclude that the uncertainty associated with the total condensate contribution \( R_0^{\text{cond}}(\tau, s_0) \) only have significant effects at high \( \tau \) regime. The condensate uncertainties (except the \( f_{cs} \) uncertainty) come from the quark condensate uncertainty, the gluon condensate uncertainty, and the uncertainties from the unknown truncated higher-dimension condensates. In the high \( \tau \) regime, the four-quark condensate has the dominant effect.

Uncertainties in perturbative part of Laplace sum rule come from the higher-loop correction to \( R_0 \) (loop \( \geq 3 \)) and even more important, come from the relatively large \( s_0 \) uncertainty. The Laplace sum rule is designed to extract information for the lowest-lying resonance in a given channel, so it is relatively insensitive to the continuum threshold \( s_0 \) value. Therefore, the uncertainty associated with \( s_0 \) is relatively large, and we conclude the perturbative part of QCD uncertainty in this thesis work mainly comes from the \( s_0 \) uncertainty. The distribution of this uncertainty with respect to \( \tau \) is shown in Figure (4.4). We find the uncertainty are large at low \( \tau \) region and negligible at the high \( \tau \).
Figure 4.3: The ratio of condensate contribution $R_0^{cond}(\tau, s_0)$ (3.87) over the total QCD sum-rule $R_0(\tau, s_0)$ (3.150) in the $I = 0$ channel. The value $s_0 = 3.5 \text{ GeV}^{-2}$ is chosen. The y-axis is the percentage value of the ratio $R_0^{cond}(\tau, s_0)/R_0(\tau, s_0)$, and the x-axis is in GeV$^{-2}$. 
end. Conservatively, perturbative uncertainties lie within 30% of total perturbative effect $R_0^{pert}(\tau, s_0)$ at the small $\tau$ range [34, 41]. Furthermore, we find that the higher-loop corrections can be understood equivalently as a change in the continuum threshold $s_0$ [117].

The instanton contributions to $R_0(\tau, s_0)$ are relatively small in the valid $\tau$ and $s_0$ region. The maximum contribution is about 10% of the total sum rule and located at the low $\tau$ regime which the perturbative uncertainty has definite dominant effect. Thus for now, the instanton uncertainty can be safely ignored in the weighting function (We have tested the variation of instanton size $\rho$, in the valid regime, and found the changed of instanton size has minor effect on the best-fit values, in both channels. the change of mass is less than 150 MeV). Its uncertainty effects will be included along with others in the Monte Carlo simulation process.

Concluding from the above uncertainty discussion and the two selecting criteria for $\epsilon(s_0, \tau)$, we find that the weighting function $\epsilon(s_0, \tau)$ must be proportional to the total $R_0(\tau, s_0)$ uncertainty, which is the sum of perturbative uncertainty and condensate uncertainty. That is:

$$\epsilon(\tau, s_0) \sim \delta R_0(\tau, s_0) = \delta R_0^{pert}(\tau, s_0) + \delta R_0^{cond}(\tau, s_0)$$  \hspace{1cm} (4.12)

From Figure (4.4) and (4.3), we notice.

$$\frac{\epsilon(\tau, s_0)}{R_0(\tau, s_0)} = \frac{\delta R_0^{pert}(\tau, s_0)}{R_0(\tau, s_0)} - \frac{\delta R_0^{cond}(\tau, s_0)}{R_0(\tau, s_0)}$$  \hspace{1cm} (4.13)

must have the shape shown in Figure (4.5).

Using the valid $\tau$ range obtained from Hölder inequality analysis (for $I = 0$ channel, $0.3 \text{GeV}^{-2} < \tau < 1.7 \text{GeV}^{-2}$), and utilizing the uncertainties estimated above, we conclude that $\frac{\epsilon(\tau, s_0)}{R_0(\tau, s_0)} = \frac{\delta R_0(\tau, s_0)}{R_0(\tau, s_0)} = 0.3$ is a conservative upper
Figure 4.4: The picture shows the relative perturbative contribution (3.44) uncertainty with respect to the change of continuum threshold $s_0$ in the $I = 0$ channel. The $s_0 = 3.5 \text{ GeV}^{-2}$ is chosen in consistent with the best-fit value. The Y-axis value is \( \left( R_0^{\text{pert}}(\tau, 4.0) - R_0^{\text{pert}}(\tau, 3.0) \right) / R_0^{\text{pert}}(\tau, 3.5) \). and the $\tau$-axis is in $\text{GeV}^{-2}$. 
Figure 4.5: Relative uncertainty on the perturbative and condensate contributions to the total QCD sum rule (3.150). $X$ axis stands for the $\tau$ range. $Y = \frac{\delta R_0(\tau, s_0)}{R_0(\tau, s_0)}$. In the valid $\tau$ range ($\tau_1 < \tau < \tau_2$) obtained from the Hölder inequality, an upper limit of the relative uncertainty always exists. The $\tau$ axis is in $GeV^{-2}$. 
limit in the valid $\tau$ range. Therefore, we identify the weighting function $\epsilon(\tau, s_0)$ as

$$\epsilon(\tau, s_0) = 0.3R_0(\tau, s_0) \quad (4.14)$$

This expression can be easily verified that it matches the two selection criteria mentioned above. As will be shown later, the coefficient of 0.3 in (4.14) is just an overall constant in the least-$\chi^2$ calculation. The change of this coefficient has no effect on the fitting procedures.

### 4.2.4 Search Algorithm

In this investigation, we will try to minimize the $\chi^2$ function.

$$\chi^2 = \frac{1}{N} \sum_{n=1}^{N} \left[ R_0(\tau_n, s_0) - aW(m, \Gamma, \tau_n)e^{-m^2\tau_n} \right]^2 / \epsilon(\tau_n, s_0)^2 \quad (4.15)$$

The parameter set to be fitted in the one resonance model is $(s_0, a, M, \Gamma)$. Our objective here is to find an optimal algorithm which will return a minimum value of $\chi^2$ when fitting the field-theoretical content in this multidimensional parameter space.

In this work, we utilize a modified version of Downhill Simplex algorithm [132] and a derivative Levenberg-Marquardt algorithm [133] to minimize the $\chi^2$ in (4.15). Comparing these two methods, we find the simplex method is superior in converging to the global minimum point in a multidimensional space. The advantage of this method is that it requires only function evaluation, but no derivatives involved. The Levenberg-Marquardt method uses derivatives to find the steepest descent step in multidimensional space. Not involving the gradient of function in the Simplex algorithm, we hope our algorithm can eas-
ily converge to the true global minimum point if several local minima exist in the very complicated multi-dimensional space.

A simplex is the geometrical figure consisting, in $N$ dimensions, of $N + 1$ points and all their interconnecting line segments, polygonal faces, etc. The downhill simplex method now takes a series steps, most of the steps just moving the point of simplex where the function is largest through the opposite face of the simplex to a lower point, and after these reflections the simplex pulls itself down in around the lowest point (the global minimum point). In our approach, the convergence is reached if the difference between the largest value point and the lowest value point in the simplex is a thousand times smaller than the average point. The above downhill simplex routine is called Amoeba. The key feature of our algorithm utilized in the QCD sum-rule analysis is to restart another Amoeba right after one Amoeba claims to find a minimum, while the initial step (i.e. the volume of the $N + 1$ point simplex) of the second Amoeba is properly chosen to give the second simplex the ability to compare one local minima with another if they exist. For example, as shown in Figure (4.6), where the function has two local minima $p_1$ and $p_2$. If the algorithm starts from point $s$, the first Amoeba will converge to local minima $p_1$ which is not a global minimum point we are searching for. By choosing a proper initial step (in this case is the distance from $p_1$ to $p_2$), the second Amoeba can initialize a simplex covering both points and eventually converge to the global minimum point $p_2$. If derivative methods such as Levenberg-Marquardt algorithm are used, the gradient of function could not tell the differences among several minima after the program leads to any of the local minimal $\chi^2$ points.

In this research, we chose $N = 20$ (divided the valid $\tau$ range into 20 evenly distributed points) to obtain the least-$\chi^2$. In practice, $N = 10$ is sufficient to give a stable estimation.
Figure 4.6: A simple two-dimension function with a local minimum point $p_1$ and a global minimum point $p_2$, where the point $s$ is supposed as the starting point.
In order to illustrate the local minima phenomena and even more importantly, to gain a quantitative approximation of the distance among local minimal points, we reduce the multidimensional space to three-dimensional space. After reducing the fitting parameters to two in the $\chi^2$ function, contour plots can be used to examine the distribution of local minima. The $\chi^2$ function defined in (4.11) is a function of four variables $\chi^2 = \chi^2(\Gamma, M, S_0, a)$. Now we fix $\Gamma$ value as an input, then the variable number is reduced to three. $\chi^2 = \chi^2(M, S_0, a)$. At local minimum, we have $\frac{\partial}{\partial a} \chi^2 \equiv 0$. and after solving this expression.

$$a = \frac{\sum_n \frac{\partial \chi^2}{\partial \tau_n} e^{-m^2 \tau_n} \cdot W[\tau_n, \Gamma, m]}{\sum_n \frac{e^{-2m^2 \tau_n} W[\tau_n, \Gamma, m]}{\Gamma \tau_n}}$$  

(4.16)

Insert the above expression back to (4.15), and set $\Gamma = 0.2 \, GeV$. we have the contour plots for $I = 0.1$ channels as shown in Figures 4.7 and 4.8.

In order to make our QCD sum-rule analysis consistent, especially the duality hypothesis of the QCD calculation above a threshold value $s_0$, we explicitly set an important criterion in our program, $m^2 \leq s_0$. This criterion will rule out certain $N$-dimension points which will contaminate the validity of Laplace sum-rule.

From Figure 4.7 and Figure 4.8, we find that in both channels there do exist several local minima, especially in $I = 1$ channel. More important, from these plots, we can roughly estimate initial steps for the second Amoeba routine in our program. this will ensure the program always converge to the global minimum point.

We compare the simplex program with the derivative Levenberg-Marquardt program explicitly with different input parameter values, and find our simplex program always converges to the global minimum least-$\chi^2$ point while the Lev-
Figure 4.7: Contour plot for the $I = 0$ channel with the input parameter values
$\Gamma = 0.2 \text{ GeV}, f_\text{es} = 1.5, \Lambda = 300 \text{ MeV},$ and $\rho = 1/(600 \text{MeV}).$
Figure 4.8: Contour plot for the $I = 1$ channel with the input parameter values
$\Gamma = 0.2 \text{GeV}$, $f_{cs} = 1.5$, $\Lambda = 300 \text{MeV}$, and $\rho = 1/(600 \text{MeV})$. 
enberg program sometimes finds only local minima.
4.3 Best-fit Analysis

4.3.1 Best-fit Results for the $I = 0, 1$ Channels

After obtaining the QCD field theory contents, the hadronic model, the valid range, the $\chi^2$ function and the suitable algorithm, we can obtain the parameter values $(m, \Gamma, s_0, a)$ which give a best fit to the Laplace sum rule $R_0(\tau, s_0)$. We employ the standard set of input values for QCD sum rule as discussed before: $\langle m\bar{q}q \rangle = -f_\pi^2m_\pi^2/2$ where $m_\pi = 140\,\text{MeV}$, $f_\pi = 93\,\text{MeV}$. $\langle \alpha_G \rangle = 0.045\,\text{GeV}^{-1}$, $\alpha(\bar{q}q)^2 = 0.00018\,\text{GeV}^{-6}$. $\Lambda = 0.3\,\text{GeV}$. $f_{\pi\pi} = 1.5$ and instanton size $\mu_0 = 1/(600\,\text{MeV})$.

Tables 4.1 and 4.2 list the lowest-resonance's parameter values as seen from a light-quark interpretation. The input parameter values are chosen to give minimum $\chi^2$ values. Our programs are designed to converge to the global minimum points starting from any point in the multi-dimensional space, so the output results are insensitive to the input values. Nevertheless, a good guess of the input values can always save substantial computational time.

Table 4.1: Best fit values for the $I = 0$ channel ($0.3\,\text{GeV}^{-2} < \tau < 1.7\,\text{GeV}^{-2}$)

<table>
<thead>
<tr>
<th>least-$\chi^2$</th>
<th>$s_0(\text{GeV}^{-2})$</th>
<th>$M(\text{GeV})$</th>
<th>$a(\text{GeV}^{-4})$</th>
<th>$\Gamma(\text{GeV})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>input</td>
<td>3.5</td>
<td>1.0</td>
<td>0.07</td>
<td>0.2</td>
</tr>
<tr>
<td>output</td>
<td>$7.758 \times 10^{-4}$</td>
<td>3.61</td>
<td>0.966</td>
<td>0.0731</td>
</tr>
</tbody>
</table>

Table 4.2: Best fit values for the $I = 1$ channel ($0.3\,\text{GeV}^{-2} < \tau < 1.1\,\text{GeV}^{-2}$)

<table>
<thead>
<tr>
<th>least-$\chi^2$</th>
<th>$s_0(\text{GeV}^{-2})$</th>
<th>$M(\text{GeV})$</th>
<th>$a(\text{GeV}^{-4})$</th>
<th>$\Gamma(\text{GeV})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>input</td>
<td>4.5</td>
<td>1.5</td>
<td>0.15</td>
<td>0.2</td>
</tr>
<tr>
<td>output</td>
<td>$2.059 \times 10^{-3}$</td>
<td>4.51</td>
<td>1.50</td>
<td>0.160</td>
</tr>
</tbody>
</table>

The best-fit gives a lowest resonance around 966 MeV in the $I = 0$ channel
and a resonance around 1500 MeV in the \( I = 1 \) channel, and both resonances have a width around 200 MeV.

In the \( I = 0 \) channel, because the 200 MeV width we obtained is substantially narrower than the 600-1200 MeV width for the \( f_0(400 - 1200) \) [50], we can conclude that \( f_0(980) \) is properly interpreted as the lowest-lying light-quark resonance in the \( I = 0 \) channel, suggesting an non-\( q\bar{q} \) interpretation of \( f_0(400 - 1200) \).

In the \( I = 1 \) channel, clearly the light-quark resonance interpretation rules out the \( a_0(980) \) as the lowest-lying resonance. The data obtained from the QCD sum-rule analysis agrees with the interpretation of the \( a_0(1450) \) as the lowest-lying \( q\bar{q} \) resonance [50]. This supports a exotica interpretation for \( a_0(980) \).

Figures (4.9) and (4.10) illustrate the fit of hadronic model with the best-fit parameter values to the QCD sum-rule \( R_\tau(\tau, s_0) \) in the \( I = 0, 1 \) channels.

### 4.3.2 Instanton Effects

We have emphasized the importance of instanton effects played in this research. They are the only terms distinguishing between the two scalar channels' QCD field-theoretical content expressions (3.150), and consequently cause the mass split between the two channels' lowest-lying resonance masses.

The QCD sum-rule is based on the quark(gluon)-hadron duality. Several authors argued that one of the most important aspects violating the duality is the existence of oscillating (exponential contribution) terms absent in the OPE calculation [35, 61], and instanton effects are responsible for the missing exponential terms in the QCD field content expression [61, 76]. Following these arguments, we expect that instanton effects should explore the oscillation feature of the missing exponential terms. Equation (3.127) does show that \( \text{Im}\Pi^{\text{inst}}(t) \sim tY_i(\sqrt{t}\rho_c)J_i(\sqrt{t}\rho_c) \), and because Bessel functions \( Y_i \) and \( J_i \)
Figure 4.9: QCD sum-rule $R_0(\tau, s_0)$ from (3.150) in the $I = 0$ channel (the solid curve) and the hadronic model with the best-fit parameters from Table 4.1 (dashed curve). The $\tau$-axis is in $GeV^{-2}$ and y-axis is in $GeV^{-4}$. 
Figure 4.10: QCD sum-rule $R_0(\tau, s_0)$ from (3.150) in the $I = 1$ channel (the solid curve) and the hadronic model with the best-fit parameters from Table 4.2 (dashed curve). The $\tau$-axis is in $GeV^{-2}$ and $y$-axis is in $GeV^{-4}$. 
Figure 4.11: The oscillating behaviour of the instanton effect (3.131) with respect to $s_0$ in the $I = 0$ channel. The $\tau$ value is fixed at 1 GeV$^{-2}$. The y-axis is in GeV$^{-4}$ and x-axis is in GeV$^{-2}$.

are oscillating, therefore the instanton effects are oscillating as well. Figures (4.11) and (4.12) do illustrate explicitly that instanton effect has an oscillating behaviour over the continuum threshold $s_0$ and $\tau$ range.

In order to illustrate the instanton effect on the mass split between the two lowest-resonance in scalar channels, the following table tabulates the results with no instanton effect in both channels. In order to make the results comparable, we choose the same $\tau$ range ($0.3 \text{ GeV}^{-2} < \tau < 1.7 \text{ GeV}^{-2}$) as the $f_0$ case.

One set of inputs we used is the same as the $I = 0$ channel best fit's
Figure 4.12: The oscillating behaviour of instanton effect (3.131) with respect to $\tau$ in the $I = 0$ channel. The $s_0$ value is fixed at $3.5 \text{ GeV}^2$ consistent with the best-fit results. The $y$-axis is in $\text{GeV}^4$ and $x$-axis is in $\text{GeV}^{-2}$. 
Table 4.3: No-instanton effect results ($0.3\, GeV^{-2} < \tau < 1.1\, GeV^{-2}$)

<table>
<thead>
<tr>
<th>input</th>
<th>output</th>
</tr>
</thead>
<tbody>
<tr>
<td>least-$\chi^2$</td>
<td>$3.32 \times 10^{-3}$</td>
</tr>
<tr>
<td>$s(0, GeV^{-2})$</td>
<td>3.5</td>
</tr>
<tr>
<td>$M(, GeV)$</td>
<td>0.2</td>
</tr>
<tr>
<td>$\alpha,(, GeV^{-4})$</td>
<td>0.15</td>
</tr>
</tbody>
</table>

input and another set used the $I = 1$ channel best fit's input. We find both inputs converge to a mass around 1.15 MeV without instanton effects. When instanton effects are included and the valid $\tau$ ranges are selected according to the inequality estimation, a mass split as large as 500 MeV occurs from the instanton effects (see the results in Table 4.1 and 4.2).

By explicit calculation, we find instanton effects are relatively large at low $\tau$ while negligible at the high $\tau$. and instanton effects have a large contribution to the total Laplace sum-rule in the $I = 1$ channel than in the $I = 0$ channel (At $\tau = 0.3\, GeV^{-2}$, the ratio $R^\text{inst}_{0}/R^\text{total}_{0} \sim 15\%$ in the $I = 1$ channel while $R^\text{inst}_{0}/R^\text{total}_{0} \sim 8\%$ in the $I = 0$ channel). Compared with the non-instanton results (Table 4.3) with the instanton-included results (Table 4.1 and 4.2) in both channels, we can conclude that the instanton effects on splitting masses between the two channels mainly from increasing the lowest-lying $I = 1$ channel's resonance mass.

Now we need to mention the instanton effect on the continuum part of the QCD sum-rule. We have found that several authors have ignored the instanton effects on the continuum part [76, 108, 114], which is the contribution to the
\[ R_0(\tau, s_0) \text{ from above } s_0, \text{ the } R_0^{cont}(\tau, s_0) \text{ can be defined as.} \]

\[
R_0(\tau, s_0) = \frac{1}{\pi} \int_0^\infty Im\Pi(t) e^{-\tau t} dt - R_0^{cont}(\tau, s_0)
\]

\[ \implies R_0^{cont}(\tau, s_0) = \frac{1}{\pi} \int_{s_0}^\infty Im\Pi(t) e^{-\tau t} dt \quad (4.17) \]

In references [76, 108, 114], the continuum contributions \( R_0^{cont} \) are calculated totally by perturbation QCD without instanton effect. Thus their instanton contributions to \( R_0(\tau, s_0) \) are equivalent to.

\[
R_0^{inst}(\tau, s_0) = \frac{1}{\pi} \int_0^\infty Im\Pi^{inst}(\tau) e^{-\tau t} dt
\]

\[
= \frac{\rho_s^2}{16\pi^2\tau^4 m^2(\tau)} e^{-\rho_s^2/(2\tau)} \left[ K_0\left(\frac{\rho_s^2}{2\tau}\right) + K_1\left(\frac{\rho_s^2}{2\tau}\right) \right] \quad (4.18)
\]

where \( K_0 \) and \( K_1 \) are the zero order and the first order Modified Bessel functions. Compared with our instanton expression (3.131).

\[
R_0^{inst}(\tau, s_0) = \frac{1}{\pi} \int_0^{s_0} Im\Pi^{inst}(\tau) e^{-\tau t} dt
\]

\[
= -\int_0^{s_0} \frac{3m^2(\tau)}{8\pi} t Y_1(\sqrt{t}\rho_c) J_1(\sqrt{t}\rho_c) e^{-\tau t} dt \quad (4.19)
\]

We find the difference between the two is a difference of

\[
\frac{1}{\pi} \int_{s_0}^\infty Im\Pi^{inst}(t) e^{-\tau t} dt. \text{ The net effects of missing instanton contributions from above the continuum threshold have a minor influence on the simulation results such as mass and } s_0. \text{ Nevertheless, it is conceptually incorrect to understand the instanton effects as in (4.18). The Hölder inequality analysis of QCD sum-rule with Eq. (4.19) form of instanton effects is shown in Figure 4.13. which verifies our argument graphically.}

Compared with Figure (4.2), we lose one of the physical features of valid
Figure 4.13: The instanton contribution $R_0^{\text{inst}}(\tau, s_0)$ to the QCD sum-rule in the $I = 0$ channel follows equation (4.19) in this figure. The input parameter values $f_{os} = 1.5$, $\Lambda = 300\,\text{MeV}$, $\rho = 1/(600\,\text{MeV}^4)$, and $\delta\tau = 0.1\,\text{GeV}^{-2}$ are used in the calculation. The $\tau$-axis is in $\text{GeV}^{-2}$ and $s_0$-axis is in $\text{GeV}^{-2}$.

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QCD sum rule inequality analysis, a global lower boundary on the continuum threshold $s_0$ in Figure (4.13). This picture indicates that at low $\tau$ regime, duality starts almost from $s_0 \sim 0$, a result that is clearly nonphysical. Globally, we don’t have a continuum threshold.

### 4.3.3 Width Effects

Now we study the finite width effects on the scalar channels. The width weighting function $W[\tau, M, \Gamma]$ is obtained via the four pulse approximation leading to equation (3.146). In order to see the effects of different width $\Gamma$ on the simulation results, we fixed the width $\Gamma$ as an input and changed its values during each simulation process, the variables in the $\chi^2$ function change to three $(s_0, M, \alpha)$.

The following tables show the simulation results.

Table 4.4: Width effects in the $I = 0$ channel, with input parameter values $s_0 = 3.5\, \text{GeV}^{-2}$, $M = 1.0\, \text{GeV}$, $\alpha = 0.07\, \text{GeV}^{-1}$, and $\tau$ range is ($0.3\, \text{GeV}^{-2} < \tau < 1.7\, \text{GeV}^{-2}$)

<table>
<thead>
<tr>
<th>input $\Gamma$ (GeV)</th>
<th>$\chi^2$</th>
<th>$s_0$ (GeV$^{-2}$)</th>
<th>$M$ (GeV)</th>
<th>$\alpha$ (GeV$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>$2.426 \times 10^{-1}$</td>
<td>3.037</td>
<td>0.854</td>
<td>0.062</td>
</tr>
<tr>
<td>0.1</td>
<td>$1.996 \times 10^{-1}$</td>
<td>3.131</td>
<td>0.872</td>
<td>0.063</td>
</tr>
<tr>
<td>0.2</td>
<td>$9.293 \times 10^{-4}$</td>
<td>3.427</td>
<td>0.930</td>
<td>0.069</td>
</tr>
<tr>
<td>0.3</td>
<td>$2.913 \times 10^{-3}$</td>
<td>3.995</td>
<td>1.046</td>
<td>0.082</td>
</tr>
<tr>
<td>0.4</td>
<td>$3.774 \times 10^{-2}$</td>
<td>4.946</td>
<td>1.257</td>
<td>0.113</td>
</tr>
<tr>
<td>0.5</td>
<td>$1.953 \times 10^{-1}$</td>
<td>6.496</td>
<td>1.608</td>
<td>0.197</td>
</tr>
</tbody>
</table>

Tables 4.4 and 4.5 indicate that the values of the lowest-lying resonance’s mass and the continuum threshold $(s_0)$ in both $I = 0, 1$ channels increase with the width $\Gamma$.

In the $I = 0$ channel, the results clearly rule out a light and broader $\sigma$ particle contributing in the lowest-lying scalar resonance. With zero-width input, the lowest-possible mass starts from 850 MeV, when the width effect
increases to 500 MeV, which is slightly comparable with the low end of the width estimated value from PDG [50] (600-1200 MeV). The mass grows to over 1600 MeV which is substantially larger than the high end of PDG [50] estimated \( \sigma \) particle's mass (400-1200 MeV). These data indicate the lowest-lying light-quark (\( \bar{q}q \)) resonance in the \( I = 0 \) channel could not be a \( \sigma \) particle. It also shows us that the lowest-lying resonance could not be \( f_0(1500) \) which has a narrow width less than 100 MeV [50], because the substantial large width (400-500 MeV) for the mass around 1500 MeV in our fixed width simulation. However, from the width effect analysis, we cannot rule out a contribution of \( f_0(1370) \) to the lowest-lying resonance in the \( I = 0 \) channel. The \( f_0(1370) \) resonance has a potential to overlap with the high-end width data in the \( I = 0 \) channel (\( f_0(1370) \) has a very large width from 200 to 500 MeV estimated by PDG). Combining the results from Tables 4.4 and 4.1, we confirm that our best-fit conclusion of \( f_0(980) \) is the lowest-lying resonance candidate in the \( I = 0 \) channel.

Table 4.5: Width effects in the \( I = 1 \) channel, with input parameter values \( s_0 = 4.5 \text{ GeV}^2, M = 1.5 \text{ GeV}, a = 0.15 \text{ GeV}^4 \), and \( \tau \) range is \( 0.3 \text{ GeV}^{-2} < \tau < 1.1 \text{ GeV}^{-2} \)

<table>
<thead>
<tr>
<th>input ( \Gamma ) (GeV)</th>
<th>( \chi^2 )</th>
<th>( s_0 ) (GeV)</th>
<th>( M ) (GeV)</th>
<th>( a ) (GeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>2.652 \times 10^{-1}</td>
<td>3.970</td>
<td>1.390</td>
<td>0.1236</td>
</tr>
<tr>
<td>0.1</td>
<td>2.515 \times 10^{-1}</td>
<td>4.095</td>
<td>1.417</td>
<td>0.1321</td>
</tr>
<tr>
<td>0.2</td>
<td>2.039 \times 10^{-1}</td>
<td>4.524</td>
<td>1.502</td>
<td>0.1613</td>
</tr>
<tr>
<td>0.3</td>
<td>1.047 \times 10^{-3}</td>
<td>5.476</td>
<td>1.649</td>
<td>0.2217</td>
</tr>
<tr>
<td>0.4</td>
<td>1.424 \times 10^{-3}</td>
<td>7.555</td>
<td>1.855</td>
<td>0.3237</td>
</tr>
<tr>
<td>0.5</td>
<td>2.575 \times 10^{-2}</td>
<td>10.97</td>
<td>2.116</td>
<td>0.4875</td>
</tr>
</tbody>
</table>

Similarly for the \( I = 1 \) channel. Table (4.5) indicates that even with zero width (the lowest possible mass case), the mass 1390 MeV is still far away from \( a_0(980) \). This further confirms our best-fit conclusion that \( a_0(1450) \) is
the lowest-lying light-quark resonance as seen from our QCD sum-rule. In this
sense, $a_0(980)$ is unnaturally decoupled from the scalar quark current, which
supports a possible $K\bar{K}$ molecule interpretation for this resonance as suggested
by [86, 114, 134].

4.3.4 Testing of Hadronic Models

As a final application of the best-fit algorithm, we test various hadronic models
and try to find the one which fits the QCD field content best, i.e. the one having
the least-$\chi^2$ value. As we have discussed in Chapter 3, there are three hadronic
models in the $I = 0, 1$ channels that should be considered:

1. One finite-width resonance model.

2. One finite-width resonance plus a finite-width excited resonance model.

3. One finite-width resonance plus a narrow-width resonance model.

Among these candidates, 1 and 2 are the most possible ones, due to the possi-
bile very large width of the lowest-lying resonance in scalar channels and the
wide nature of excited state resonances (generally speaking, excited states are
less stable than ground states). However, we test all of the three candidates
explicitly in the $I = 0$ channel.

The one finite width model is nothing but the best fit results from Table
4.1, while the two finite-width resonance model is defined as

$$Model = a_1 W^\dagger_1 m_1 \cdot \Gamma_1 \cdot \tau e^{-m_1^2 \tau} + a_2 W^\dagger_2 m_2 \cdot \Gamma_2 \cdot \tau e^{-m_2^2 \tau} \quad (4.20)$$

Equating the hadronic model to the QCD sum rule $R_0(\tau, s_0)$ and follow the
same form of $\chi^2$ function, we have 7 parameters $(s_0, a_1, \Gamma_1, m_1, a_2, \Gamma_2, m_2)$ to
fit. Observe the different candidate resonances existing in the $I = 0$ channel
[50], we find the possible two subcontinuum resonances must be one around 980 MeV another one around 1500 MeV, thus we use these two numbers as our initial input guess.

Table 4.6: Two finite-width resonance model with same input values

<table>
<thead>
<tr>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>least-χ²</td>
<td>8.64 × 10⁻⁴</td>
</tr>
<tr>
<td>s₀(GeV⁻²)</td>
<td>3.5</td>
</tr>
<tr>
<td>a₁(GeV⁻¹)</td>
<td>0.07</td>
</tr>
<tr>
<td>m₁(GeV)</td>
<td>1.0</td>
</tr>
<tr>
<td>Γ₁(GeV)</td>
<td>0.2</td>
</tr>
<tr>
<td>a₂(GeV⁻¹)</td>
<td>0.07</td>
</tr>
<tr>
<td>m₂(GeV)</td>
<td>1.0</td>
</tr>
<tr>
<td>Γ₂(GeV)</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Table 4.6 indicates the two resonances converge to the same mass around 980 MeV. Compared with Table 4.1, the only effect of the two finite-width resonance model is the split of coupling coefficient a between a₁ and a₂.

Table 4.7: Two finite-width resonance model with different input values

<table>
<thead>
<tr>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>least-χ²</td>
<td>7.30 × 10⁻⁴</td>
</tr>
<tr>
<td>s₀(GeV⁻²)</td>
<td>3.5</td>
</tr>
<tr>
<td>a₁(GeV⁻¹)</td>
<td>0.07</td>
</tr>
<tr>
<td>m₁(GeV)</td>
<td>1.0</td>
</tr>
<tr>
<td>Γ₁(GeV)</td>
<td>0.2</td>
</tr>
<tr>
<td>a₂(GeV⁻¹)</td>
<td>0.07</td>
</tr>
<tr>
<td>m₂(GeV)</td>
<td>1.5</td>
</tr>
<tr>
<td>Γ₂(GeV)</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Table 4.7 use different mass values as input, the output results do not show two clearly distinguished resonances below the continuum threshold. One resonance is centered at 830 MeV with a 175 MeV width largely overlapped.
with another resonance centered at 1120 MeV with a 239 MeV width. Besides
we observe the least-$\chi^2$ value in this model is the same order of magnitude
as that from one finite-width model shown in Table 4.1. Identification of the
830 MeV and 1120 MeV as two separate resonances is in contradiction with
the results of the leading $I = 1$ pseudoscalar current sum rule, for which a
fit including two contributing subcontinuum resonances ($\pi$ and $\pi'$) leads to a
$\chi^2$ an order of magnitude lower than of a single resonance fit [116]. Thus we
can safely conclude the two finite-width resonance model gives one finite width
subcontinuum resonance as output of our program.

For the one finite plus a narrow resonance model, we write the hadronic
ansatz as

$$Model = a_1 W[m_1, \Gamma_1, \tau] e^{-m_1^2\tau} + a_2 e^{-m_2^2\tau}$$  \hspace{1cm} (4.21)

Knowing the results of one and two finite-width resonance models, we can
conclude the width is around 200 MeV, so we fix this value as an input in the
program. Thus, this model has five parameters ($s_0, a_1, m_1, a_2, m_2$) to fit the
QCD sum rule $R_0(\tau, s_0)$

Table 4.8: One finite-width plus a narrow resonance model with input width
$\Gamma = 0.2 GeV$

<table>
<thead>
<tr>
<th></th>
<th>input</th>
<th>output</th>
</tr>
</thead>
<tbody>
<tr>
<td>least-$\chi^2$</td>
<td>$8.57 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>$s_0(\text{GeV}^{-2})$</td>
<td>3.5</td>
<td>3.51</td>
</tr>
<tr>
<td>$a_1(\text{GeV}^{-4})$</td>
<td>0.07</td>
<td>0.067</td>
</tr>
<tr>
<td>$m_1(\text{GeV})$</td>
<td>1.0</td>
<td>0.924</td>
</tr>
<tr>
<td>$a_2(\text{GeV}^{-4})$</td>
<td>0.07</td>
<td>0.0035</td>
</tr>
<tr>
<td>$m_2(\text{GeV})$</td>
<td>1.5</td>
<td>1.359</td>
</tr>
</tbody>
</table>
Comparing the coupling coefficients of the two output resonances centered at 924 MeV and 1340 MeV respectively, we find that the narrow higher mass resonance couples to the light quark current \((a_2)\) 20 times smaller than that of the finite width resonance at 935 MeV \((a_1)\). Thus, the excited-state contribution is totally negligible, and we can conclude only one finite resonance exists in this model. As before, the \(\chi^2\) is not substantially reduced compared to the single resonance model.

Summarizing the conclusions from the above three hadronic models, we can state that the leading \(I = 0\) scalar-current sum-rule is dominated by a single finite-width resonance. The same conclusion applies to the \(I = 1\) channel.
4.4 Uncertainty Estimation: Monte-Carlo Simulations

One of the common shortcomings in traditional QCD sum rule analysis is claiming a accuracy statement for QCD sum rule prediction without supporting calculations. Even with a stability analysis, not all parameters' uncertainties are considered simultaneously. These are the problems we are trying to avoid in this section.

In this section, we will estimate the uncertainties of the least-$\chi^2$ analysis method originating from various uncertainty sources in the QCD parameters employed in the sum rule calculation. We will seek the combined effects of all these uncertainties integrated together, not simply individual QCD parameter variations. In this way, we will learn how the uncertainties in QCD parameters are mapped into uncertainties in the phenomenological fit parameters.

The standard values and the associated uncertainties of the free parameters used in this analysis ($\Lambda$, $f_{vs}$, $\langle \bar{q}q \rangle$, $\langle \alpha GG \rangle$, $\langle \alpha \bar{q}q \bar{q}q \rangle$, $s_0$, and $\rho_c$) have been discussed earlier. The uncertainties related to $s_0$ (the continuum uncertainty), $\langle \bar{q}q \rangle$, $\langle \alpha GG \rangle$, $\langle \alpha \bar{q}q \bar{q}q \rangle$ are combined together into the weighting function $\epsilon(\tau, \tau_0)$ in the $\chi^2$ formulation, which is 30% of total Laplace sum rule $R_\theta(\tau, \tau_0)$. The vacuum saturation factor $f_{vs}$ can vary from 1 to 2 and instanton size has a 15% uncertainty. Figures (4.14) and (4.15) show the combinations of power law and continuum uncertainties. i.e. $\epsilon(\tau, s_0) = 0.3R_\theta(\tau, s_0)$, are well defined by the following empirical formula. The $R_\theta(\tau, s_0)$ is enumerated at the best-fit values ($\Lambda = 0.3$ GeV, $f_{vs} = 1.5$).

1. For the $I = 0$ case, the input $s_0 = 3.5$ GeV$^{-2}$, $\epsilon(\tau) = a_1\exp(-1.05015\tau^{-0.7326})$ where $a_1 = 0.01714$ GeV$^{-4}$.

2. For the $I = 1$ case, the input $s_0 = 4.5$ GeV$^{-2}$, $\epsilon(\tau) = a_2\tau\exp(-5.74705\tau^{0.5267})$ where $a_2 = 1.1547$ GeV$^{-4}$.
Figure 4.14: The weighting function $\epsilon(\tau, s_0)$ from (4.14) in the $I = 0$ channel (the dashed curve) and the empirical model shown as the solid curve. The y-axis is in $GeV^{-1}$ and x-axis is in $GeV^{-2}$.

The simulation of the uncertainties of the continuum part and condensates contribution is through the random variation of $a_1$ and $a_2$ in the above two empirical expressions. $a_1$ and $a_2$ are constrained to regions

$-0.01714 GeV^{-1} < a_1 < 0.01714 GeV^{-1}$, $-1.1547 GeV^{-1} < a_2 < 1.1547 GeV^{-1}$

so that the simulation does not exceed the error estimation of $R_0(\tau, s_0)$.

Now we can conduct the uncertainty estimation by performing a Monte-Carlo simulation with random variation in the parameter set $(\rho, a_1, a_2$ and
Figure 4.15: The weighting function $\varepsilon(\tau, s_0)$ from (4.14) in the $I = 1$ channel (the dashed curve) and the empirical model shown as the solid curve. The y-axis is in $GeV^{-4}$ and x-axis is in $GeV^{-2}$. 
\[ \frac{0.85}{600 \, MeV^2} < \rho_e < \frac{1.15}{600 \, MeV^2} \]
\[ -0.01714 \, GeV^{-4} < a_1 < 0.01714 \, GeV^{-4} \]
\[ -1.1547 \, GeV^{-4} < a_2 < 1.1547 \, GeV^{-4} \]
\[ 1 < f_{vs} < 2 \]
(4.22)

The criterion \((M^2 < s_0)\) discussed in the best-fit simulation is still employed to make the Monte-Carlo simulation consistent with the duality hypothesis.

In practice, 500 point simulations are performed in each channel; however, a 100 point simulation is sufficient to get a stable uncertainty estimation. The following figures are the histograms plots of the fitted parameter from the 500 simulations in both cases.

From Figures (4.16), (4.17), (4.18) and (4.19), we find the masses are nicely centered around the best-fit value \((m_{I=0} = 1000 \, MeV, \ m_{I=1} = 1500 \, MeV)\) with a relatively narrow region of uncertainty space in both scalar channels. while the values for \(s_0\) vary across a relatively large uncertainty space (in the \(I = 0\) channel \(3.0 \, GeV^{-2} < s_0 < 4.5 \, GeV^{-2}\), in the \(I = 1\) channel \(4.0 \, GeV^{-2} < s_0 < 6.5 \, GeV^{-2}\)). This should not be suppressing because Laplace sum rules are designed to be sensitive to lowest-lying resonance's contribution, and they give a relatively larger uncertainty prediction on the continuum threshold value.

The 90% confidence level interval 500-point Monte-Carlo simulation results are presented in Tables 4.9 and 4.10.

For the \(I = 0\) channel, we find a mass with a central value 1000 MeV and an average width of 193 MeV, ruling out the possibility of \(f_0(1370)\) (according to [50]. \(f_0(1370)\) has a mass \(1200 \rightarrow 1500 \, MeV\) with a \(200 \rightarrow 500 \, MeV\) width) as a dominant contribution to the lowest-lying light-quark resonance in QCD.
Figure 4.16: Histogram for the $f_0$ mass obtained from fits of 500 parameter sets.
Figure 4.17: Histogram for the $f_0$ continuum threshold obtained from fits of 500 parameter sets. The continuum threshold value is in $GeV^2$. 
Figure 4.18: Histogram for the $a_0$ mass obtained from fits of 500 parameter sets.
Figure 4.19: Histogram for the $a_0$ continuum threshold obtained from fits of 500 parameter sets. The continuum threshold value is in $GeV^2$. 
Table 4.9: Monte Carlo simulation results for the $I = 0$ channel ($0.3 \text{GeV}^{-2} < \tau < 1.7 \text{GeV}^{-2}$)

<table>
<thead>
<tr>
<th></th>
<th>$s_0(\text{GeV}^2)$</th>
<th>$M(\text{GeV})$</th>
<th>$a(\text{GeV}^{-1})$</th>
<th>$\Gamma(\text{GeV})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>input</td>
<td>3.5</td>
<td>1.0</td>
<td>0.07</td>
<td>0.2</td>
</tr>
<tr>
<td>output</td>
<td>$3.73 \pm 0.45$</td>
<td>$1.000 \pm 0.087$</td>
<td>$0.079 \pm 0.023$</td>
<td>$0.19 \pm 0.14$</td>
</tr>
</tbody>
</table>

Table 4.10: Monte Carlo simulation results for the $I = 1$ channel ($0.3 \text{GeV}^{-2} < \tau < 1.1 \text{GeV}^{-2}$)

<table>
<thead>
<tr>
<th></th>
<th>$s_0(\text{GeV}^2)$</th>
<th>$M(\text{GeV})$</th>
<th>$a(\text{GeV}^{-1})$</th>
<th>$\Gamma(\text{GeV})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>input</td>
<td>4.5</td>
<td>1.5</td>
<td>0.15</td>
<td>0.2</td>
</tr>
<tr>
<td>output</td>
<td>$4.95 \pm 0.72$</td>
<td>$1.55 \pm 0.11$</td>
<td>$0.170 \pm 0.035$</td>
<td>$0.22 \pm 0.11$</td>
</tr>
</tbody>
</table>

sum rule. It is also definitely not a $\sigma$-like particle which needs a light and broader structure, and the best fit simulation (Table 4.1) rules out a dominant contribution of $f_0(1500)$ as the lowest-lying resonance. Therefore, together with the best-fit results, we confirm again that the lowest-lying resonance in the $I = 0$ channel is the $f_0(980)$ with a light-quark interpretation.

For the $I = 1$ channel, without any question, the lowest-lying resonance is $a_0(1450)$. The $a_0(980)$ must be unnaturally decoupled from the light-quark current suggesting an exotica structure can be used to interpret the $a_0(980)$.

The width ranges obtained from Monte-Carlo simulation for the two scalar channels ($50 \text{MeV} < \Gamma_{I=0} < 330 \text{MeV}, 110 \text{MeV} < \Gamma_{I=1} < 330 \text{MeV}$) are also consistent with the above two conclusions ($f_0(980)$ and $a_0(1450)$ are the lowest-lying resonances). From Table 2.3, the PDG estimated values for the two mesons are $40 \text{MeV} < \Gamma < 100 \text{MeV}$ for $f_0(980)$ and $252 \text{MeV} < \Gamma < 278 \text{MeV}$ for $a_0(1450)$ are embedded in the Monte-Carlo estimations.

The much higher $I = 1$ value for the continuum threshold in Table 4.10 is comparable to the values for $s_0$ obtained via sum rule analysis of the $I = 1$
The pseudoscalar channel [117, 131]. In both $I = 0.1$ channels, sum rule methodology would suggest that Borel stability not occur for values of $s_0^{1/2}$ that are less than the masses of contributing subcontinuum resonances. The large value of mass evident from Table 4.10 necessarily requires values of $s_0$ larger that of the $I = 0$ channel, consistent with the values of $s_0$ actually listed.

As mentioned before, the Hölder inequality provides a valuable criterion for studying the validity and self-consistency of a QCD sum-rule calculation. Not all QCD sum rules are consistent with Hölder inequality constraints. Inconsistencies between QCD sum-rule calculations and Hölder inequalities have been found in the literature [131], which indicates those QCD sum-rule calculations do not consistently describe integrated physical cross-sections, i.e. those calculations could not provide a convincing description of a resonance and physical continua. Therefore, it is worth checking our simulation results with Hölder inequalities. Comparing the $s_0$ values obtained from our Monte-Carlo simulations (for the $I = 0$ channel, $3.28 \text{ GeV}^2 < s_0 < 4.18 \text{ GeV}^2$: for the $I = 1$ channel $4.23 \text{ GeV}^2 < s_0 < 5.67 \text{ GeV}^2$) with Figure (4.1) and Figure (4.2), we find the above two $s_0$ Monte-Carlo estimated values lie within the corresponding valid $s_0 - \tau$ region from Hölder inequality analysis. Thus we conclude that our least-$\chi^2$ simulation results are consistent with Hölder inequality constraints on the corresponding channel's QCD sum-rule.
Chapter 5

Conclusions

The goal of this thesis is determining which of several empirically justifiable interpretations of the experimental observed resonances in the scalar channels are compatible with theoretical constraints based on QCD sum-rule methodology.

Compared with traditional derivative sum-rule ratio methods, we find that the least-$\chi^2$ extraction of the properties of the lowest-lying scalar mesons, obtained from a global fit to the shape of the fundamental QCD Laplace sum rule of the light-quark non-strange currents, has several reliability and validity advantages. To calculate the least-$\chi^2$, a modified version of the Downhill simplex algorithm is employed. Compared explicitly with the derivative Levenberg-Marquardt algorithm, we find that the no-derivative-involved simplex method is superior in converging to the global minimum point provided some preliminary knowledge is gained about the rough separations among local minima.

One of the unique features of this thesis is the utilization of the Hölder inequality technique to determine the valid Borel scale $\tau$ range for our QCD sum-rule analysis. The Hölder inequality provides fundamental constraints for the QCD sum-rule to consistently describe integrated physical cross-sections. With no need for any phenomenological inputs, the Hölder inequality supplies a rigorous method for determining the valid $\tau$ range and $s_0$ space for a given QCD sum-rule.

The single-instanton contribution is incorporated in the field theoretical content of the scalar QCD sum rules. Instanton effects are of ultimate important in this study since they are the only distinct components in the $I = 0, 1$ channel's QCD sum rules to any loop order. Therefore instantons are respon-
sible for breaking the mass degeneracy between the lowest-lying isovector and isoscalar mesons. A novel treatment of instanton effects in the QCD continuum contribution is developed in this thesis. The Hölder inequality analysis shows that the widely accepted formula for instanton effects is incorrect.

A four-pulse approximation finite width effect is incorporated into the hadronic contribution of QCD Laplace sum rules to overcome the narrow resonance model's limits in study the lowest-lying scalar resonance properties. From the best-fit simulation results, we find a lowest-lying resonance's finite-width effect elevates a sum-rule determination of that resonance's mass. Several possible hadronic models are explicitly tested, and we conclude that the scalar rum rules are dominated by a single finite-width resonance.

The best-fit gives a lowest-lying resonance around 966 MeV in the $I = 0$ channel and a lightest resonance around 1500 MeV in the $I = 1$ channel. Both resonance's widths are around 200 MeV. These results indicate $a_0(1450)$ being the lowest-lying $\bar{q}q$ meson in the $I = 1$ channel, suggesting an exotic interpretation of the $a_0(980)$. In the $I = 0$ channel, the results clearly rule out a dominant contribution of the $f_0(400-1200)$ to the light quark current's sum-rule, and the $f_0(980)$ is identified as the lowest-lying $\bar{q}q$ isoscalar resonance.

The stability analyses of the QCD sum-rule best-fit predictions are conducted through a Monte-Carlo simulation based on the uncertainties of the perturbative contribution, the instanton contribution, the condensate contribution, and the vacuum saturation hypothesis. The results of the fitting procedure at 90% confidence level are as follows: For the $I = 0$ channel, the lowest-lying resonance's mass is $M = (1.000 \pm 0.087) \text{GeV}$, the total width is $\Gamma = (0.19 \pm 0.14) \text{GeV}$, the corresponding continuum threshold is $s_0 = (3.73 \pm 0.45) \text{GeV}^2$ and the resonance's coupling coefficient is $a = (0.079 \pm 0.023) \text{GeV}^{-4}$. For the $I = 1$ channel, the results are $M = (1.55 \pm 0.11) \text{GeV}$, $\Gamma = (0.22 \pm$
0.11) GeV. $s_0 = (4.95 \pm 0.72) \text{GeV}^2$ and $a = (0.170 \pm 0.035) \text{GeV}^4$. These results are in good agreement with the best-fit predictions and consistent with the Hölder inequality constraints.

In conclusion, $f_0(980)$ is identified as the lowest-lying light quark resonance from our QCD sum-rule analysis in the $I = 0$ channel. This conclusion is supported by [85, 87, 89]. The $f_0(400-1200)$ is unnaturally decoupled from a light quark current, we suggest a glueball or a mixture of glueball and quarkonium structure for this controversial $\sigma$ meson [135]. An in-depth study of this possibility is in progress in our research group. In the $I = 1$ channel, we conclude that $a_0(1450)$ is the lightest $\bar{q}q$ resonance. This indicates a non-$\bar{q}q$ structure for $a_0(980)$, and hence a $K^*\bar{K}$-molecule structure for this resonance is preferred [86, 87].
References

[16] W. Heisenberg. W. Pauli. Z. Phys. 56 (1929) 1
            New York 1966
            Addison-Wesley, Cambridge 1995

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[78] M. Gell-Mann, Phys. Rev. 92 (1953) 833


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Appendix A
Conventions and Notations

In this thesis, natural units are employed.

\[ h = c = 1. \quad 1 \sim 200 \text{MeV} \cdot F \quad (A.1) \]

In these units, the position in a contravariant coordinate is denoted by a 4-vector \( x^\mu \).

\[ x^\mu = (x^0, x^1, x^2, x^3) = (t, x, y, z) = (t, \vec{r}) \quad (A.2) \]

The covariant coordinate \( x_\mu \) is defined by

\[ x_\mu = g_{\mu\nu}x^\nu = (t, -\vec{r}) \quad (A.3) \]

where the matrix \( g_{\mu\nu} \) defines as

\[ g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (A.4) \]

The Minkowski space matrix is defined by the following line element.

\[ ds^2 = dx^\mu dx_\mu = g^{\mu\nu}dx_\mu dx^\nu = dt^2 - (d\vec{r})^2 \quad (A.5) \]

where the Einstein summation convention of “sum over repeated indices” is followed.

In the \( h = c = 1 \) units system, the Lagrangian for free Dirac fermion of mass \( m \) is

\[ \mathcal{L}(x) = \bar{\psi}(x) \left( i\gamma^\mu \partial_\mu - m \right) \psi(x) \quad (A.6) \]

where the \( \gamma_\mu \) are the \( 4 \times 4 \) Dirac matrices satisfy the algebra

\[ \{ \gamma^\mu, \gamma^\nu \} = \gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu} \quad (A.7) \]

\[ \gamma^\mu = g^{\mu\nu} \gamma_\nu, \quad \gamma^0 = (\gamma^0, \vec{\gamma}) \quad (A.8) \]

\[ \gamma_\mu = (\gamma_0, -\vec{\gamma}). \quad \gamma^5 = \gamma_5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3 \quad (A.9) \]
A common notation is \( \gamma = a^a \gamma^a \).

The Dirac representation of the \( \gamma \) matrices is defined as.

\[
\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \gamma^3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}
\]

(A.10)

where the \( I \) in the above equation is a \( 2 \times 2 \) unit matrix \( \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \). The \( \sigma \) matrices are the Pauli matrices

\[
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

(A.11)

The eight traceless generators \( \lambda \) of \( SU_c(3) \) group are called the \( 3 \times 3 \) Gell-Mann matrices.

\[
\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}
\]

(A.13)

\[
\lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}
\]

(A.14)

\[
\lambda_5 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}
\]

(A.15)

\[
\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}
\]

(A.16)

The general representations \( T^a \) of \( SU_c(3) \) obey a Lie algebra

\[
T^a = 2\lambda^a, \quad Tr[T^a] = 0
\]

(A.18)

\[
[T^a, T^b] = T^a T^b - T^b T^a = i f_{abc} T^c
\]

(A.19)

\[
f_{abc} = -f_{bac} = -f_{acb}
\]

(A.20)

where the anti-symmetric \( f_{abc} \) are known as the Lie group structure constants.
Appendix B
Example REDUCE Program

The following is an example REDUCE program used in calculating the gluon condensate contribution to the light-quark scalar current correlation function. This calculation corresponds to the third plot in Figure (3.4) in Chapter 3.

The indented lines are the actual REDUCE codes and the others are the output.

REDUCE 3.4.1, 15-Jul-92 ...

> off allfac;

>

> vecdim 4+2*ep;

>

>

> vector q,p,p1,p2,p3;

>

> vector v,tau,la,rho;

>

>

> for all y let gamma(y)=1/y-r+1/2*(r*r+z)*y;

*** gamma declared operator

>

> for all y let gamma1(y)=y*gamma(y);

*** gamma1 declared operator

>

> for all y let gamma2(y)=(1+y)*gamma1(y);

*** gamma2 declared operator

>

>

> for all y let gamma3(y)=(2+y)*gamma2(y);
*** gamma3 declared operator

> >
> for all y let ngamma1(y)=1/(-1+y)*gamma(y);

*** ngamma1 declared operator

> >
> for all y let ngamma2(y)=1/(-2+y)*ngamma1(y);

*** ngamma2 declared operator

> >
> for all y let ngamma3(y)=1/(-3+y)*ngamma2(y);

*** ngamma3 declared operator

> >
> >
> >
> >
> > for all p let fp(p)=i*(g(l,p))/(p.p);

*** fp declared operator

> >
> for all p let vcg(p)=-i*g*g(l,p);

*** vcg declared operator

> >
> let p1.p1=x, p2.p2=y, p3.p3=z, (p1-q).(p1-q)=w;

> >
> let q.q=q2, p1.q=-(w-q2-x)/2;

> >
> >
> > ampl:=fp(p1)*vcg(rho)*fp(p2)*g(1,tau)*fp(p2)*fp(p3)*g(1,v)*fp(p3)*vcg(1a)*fp(f

> >
> let p2=p1;

> let p3=p1-q;
> let y=x;
> let z=w;
>
> index v,tau,la,rho;
>
> amps:=(v.tau*la.rho-v.rho*la.tau)*ampl;

\[
amps := ( -4*ep*g*q2 + 4*ep*g*w + 4*ep*g*x - 10*ep*g*q2
\]
\[
+ 10*ep*g*w + 10*ep*g*x - 6*g*q2 + 6*g*w + 6*g*x)/(w^2*x)
\]

> remind v,tau,la,rho;
>
> let denp=(x*w)**8;
>
> ampl:=amps*denp$
>
> for all m,n match x**m*w**n=fi(8-m,8-n);
>
> amps:=ampl;

*** fi declared operator

\[
amps := -4*fi(2,2)*ep*g*q2 - 10*fi(2,2)*ep*g*q2 - 6*fi(2,2)*g*q2 + 4*fi(2,1)*ep*g + 10*fi(2,1)*ep*g + 6*fi(2,1)*g + 4*fi(1,2)*ep*g + 10*fi(1,2)*ep*g
\]

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\[ 2 + 6 \cdot \text{fi}(1,2) g \]

\[
> \>
> \text{let fi}(2,3) = 1/16 / \pi / \pi / q^2 \cdot 3 \cdot \text{gamma}(ep) \cdot \text{ngamma}1(ep) \cdot \text{gamma}3(-ep) / 2 / \text{ngamma}1(2*ep); \\
> \text{let fi}(2,2) = 1/16 / \pi / \pi / q^2 \cdot 2 \cdot \text{gamma}(ep) \cdot \text{gamma}(ep) \cdot \text{gamma}2(-ep) / \text{gamma}(2*ep); \\
> \text{let fi}(2,1) = 1/16 / \pi / \pi / q^2 \cdot \text{gamma}(ep) \cdot \text{gamma}1(ep) \cdot \text{gamma}1(-ep) / \text{gamma}(2*ep); \\
> \text{let fi}(1,3) = 1/16 / \pi / \pi / q^2 \cdot 2 \cdot \text{gamma}1(ep) \cdot \text{ngamma}1(ep) \cdot \text{gamma}2(-ep) / 2 / \text{gamma}(2*ep); \\
> \text{let fi}(1,2) = 1/16 / \pi / \pi / q^2 \cdot \text{gamma}(ep) \cdot \text{gamma}(ep) \cdot \text{gamma}1(-ep) / \text{gamma}(2*ep); \\
> \text{let fi}(0,3) = 0;
\]

\[
\text{ampl} := \text{amps};
\]

<table>
<thead>
<tr>
<th>8 2 6</th>
<th>8 2 4</th>
<th>8 2 2 2</th>
<th>8 2 3</th>
</tr>
</thead>
</table>

\[
\text{ampl} := (2*ep \cdot g \cdot r + 6*ep \cdot g \cdot r \cdot w + 6*ep \cdot g \cdot r \cdot w + 2*ep \cdot g \cdot w
\]

<table>
<thead>
<tr>
<th>7 2 5</th>
<th>7 2 5</th>
<th>7 2 4</th>
</tr>
</thead>
</table>

\[
+ 5*ep \cdot g \cdot r - 4*ep \cdot g \cdot r + 15*ep \cdot g \cdot r \cdot w
\]

<table>
<thead>
<tr>
<th>7 2 3</th>
<th>7 2 2 2</th>
<th>7 2 2</th>
</tr>
</thead>
</table>

\[
- 8*ep \cdot g \cdot r \cdot w + 15*ep \cdot g \cdot r \cdot w - 4*ep \cdot g \cdot r \cdot w
\]

<table>
<thead>
<tr>
<th>7 2 3</th>
<th>6 2 6</th>
<th>6 2 5</th>
<th>6 2 4</th>
</tr>
</thead>
</table>

\[
+ 5*ep \cdot g \cdot w + 3*ep \cdot g \cdot r - 10*ep \cdot g \cdot r + 9*ep \cdot g \cdot r \cdot w
\]

<table>
<thead>
<tr>
<th>6 2 4</th>
<th>6 2 3</th>
<th>6 2 2 2</th>
</tr>
</thead>
</table>

\[
+ 4*ep \cdot g \cdot r - 20*ep \cdot g \cdot r \cdot w + 9*ep \cdot g \cdot r \cdot w
\]

| 16*ep \cdot g \cdot r \cdot w - 10*ep \cdot g \cdot r \cdot w + 3*ep \cdot g \cdot w
|-------|-------|-------|

<table>
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<th>6 2 2</th>
<th>5 2 5</th>
<th>5 2 4</th>
</tr>
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</table>

\[
+ 12*ep \cdot g \cdot w - 6*ep \cdot g \cdot r + 10*ep \cdot g \cdot r
\]

<table>
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<tr>
<th>5 2 3</th>
<th>5 2 2</th>
<th>5 2 2</th>
</tr>
</thead>
</table>

\[
- 12*ep \cdot g \cdot r \cdot w + 40*ep \cdot g \cdot r \cdot w - 6*ep \cdot g \cdot r \cdot w
\]

185
5 2 5 2 2 4 2 4
- 16*ep *g *r*w + 30*ep *g *w + 6*ep *g *r

4 2 2 4 2 2 4 2
+ 24*ep *g *r *w + 8*ep *g *r - 40*ep *g *r*w

4 2 2 4 2 3 2 2 3 2
+ 18*ep *g *w + 24*ep *g *w + 20*ep *g *r - 24*ep *g *r*w

3 2 3 2 2 2 2 2 2
- 16*ep *g *r + 50*ep *g *w + 12*ep *g *r - 40*ep *g *r

2 2 2 2 2 2 2
+ 36*ep *g *w + 16*ep *g - 24*ep*g *r + 40*ep*g + 24*g )/

2 2 2 2 2 2 2
(64*ep *pi *q2*r + 64*ep *pi *q2*w - 64*ep*pi *q2*r

2
+ 32*pi *q2)

> amps:=sub(ep=0, df(*ep*ep*ampl, ep, 2 ));

2
3*g
amps := ---------------
2
4*pi *q2

>