Inverse Problem Approach for Non-Perturbative QCD: Foundation

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Abstract

We propose a novel theoretical framework to calculate the non-perturbative QCD quantities. It starts from the dispersion relation of quantum field theory, separating the high-energy and low-energy scales and using the known perturbative theories to solve the unknown non-perturbative quantities by the inverse problem. We prove that the inverse problem of dispersion relation is ill-posed, with unique but unstable solutions. The regularization methods must be used to get the stable approximate solutions. The method is based on the strict mathematics, without any artificial assumptions. We have test some toy models to vividly show the main features of the inverse problem. It can be found that this approach can systematically improve the precision of the solutions.

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1 Introduction

How to precisely calculate the non-perturbative quantities is one of the most important problems in particle physics and nuclear physics. It is closely connected to understand the low-energy dynamics of strong interaction and the color confinement. Besides, the indirect search for the new physics beyond the Standard Model is also related to the non-perturbative calculations, since the main theoretical uncertainties always come from the non-perturbative hadronic quantities, such as the hadronic vacuum polarization in the muon \( g - 2 \).

The current non-perturbative methods include the Lattice QCD, the QCD (light-cone) sum rules, the Dyson-Schwinger Equation, the chiral perturbative theory, and some effective field theories or phenomenological models. Each of them has its advantages and disadvantages. A new method of non-perturbative calculations is always welcomed.

In [1], a novel method was firstly proposed in the studies of \( D^0 - \bar{D}^0 \) mixing, using the high-energy perturbative theories to calculate the low-energy non-perturbative quantities by solving the inverse problem of dispersion relations. But the mathematical structure of this method was unclear, which is one of the main purpose of this work. Later on, the collaborators of one of author of this paper continue to apply this approach to study more physical problems, such as muon \( g - 2 \) [2], modifying the QCD sum rules [3], the Glueballs [4], the pion distribution amplitudes [5] and neutral meson mixings [6].

In this work, we systematically develop the theoretical framework of the inverse problem approach. The main ideas of the inverse problem approach are as follows. It starts from the dispersion relation of quantum field theory, separating the high-energy and low-energy scales and using the known perturbative
theories to solve the unknown non-perturbative quantities by the inverse problem. We prove that the inverse problem of dispersion relation is ill-posed, with unique but unstable solutions. The regularization methods must be used to get the stable approximate solutions. The method is based on the strict mathematics, without any artificial assumptions. We have test some toy models to vividly show the main features of the inverse problem. It can be found that this approach can systematically improve the precision of the solutions.

2 Inverse Problem of Dispersion Relation

The dispersion relations is widely used in particle physics, nuclear physics, chiral perturbation theory, QCD sum rules and so on.

Starting from a correlation function of \( \Pi(q^2) = i \int d^4x e^{iqxt} \langle O(x)O(0) \rangle \), the dispersion relation can be easily obtained as

\[
\Pi(q^2) = \frac{1}{\pi} \int_{s_{\text{min}}}^{\infty} ds \frac{\text{Im} \Pi(s)}{s - q^2 - i\epsilon},
\]

or equally as

\[
\text{Re}[\Pi(s)] = \frac{1}{\pi} P \int_0^{\infty} \frac{\text{Im} [\Pi(s')]}{s - s'} ds'.
\]

Split the right-hand side of the equation (2.2) in two parts by a scale \( \Lambda \) separating the high-energy perturbative physics and the low-energy non-perturbative ones, and get the following form:

\[
P \int_0^{\Lambda} \frac{\text{Im} [\Pi(s')]}{s - s'} ds' = \pi \text{Re}[\Pi(s)] - P \int_{\Lambda}^{\infty} \frac{\text{Im} [\Pi(s')]}{s - s'} ds'.
\]

The integrand \( \text{Im} \Pi(s') \) in the left-hand side of equation (2.3) is unknown, which collects nonperturbative contributions form the low \( s \) region, and the right-hand of equation (2.3) can be calculated by perturbation theory clearly. So we want get all the nonperturbative contributions by solving the integral equation (2.3).

We simplify the equation (2.3) to the following operator equation and see it as an inverse problem:

\[
K f = \int_a^b \frac{f(x)}{y - x} dx = g(y), \quad y \in [c, d], f \in F, g \in G,
\]

where \( K \) is an operator from Hilbert space \( F = L^2(a, b) \) to Hilbert space \( G = L^2(c, d) \). Selecting different spaces \( F, G \) will lead to different mathematical properties of the inverse problem (2.4) [8] while the \( L^2 \) space is enough to research in this study. The integral equation (2.4) is called the Fredholm integral equation of the first kind [9]. Besides, we set \( d > c > b > a \geq 0 \) which reason is to decrease difficulties to solve the inverse problem by eliminating singularity of the integral equation (2.4).
3  Ill-posedness of the inverse problem

Inverse problems have been studied widely on both respects of mathematical analysis and numerical computations motivated by their various applications in science and technology, such as medical imaging, nondestructive testing, geological prospecting, computer tomography, and inverse scattering, etc. One problem is called an inverse problem, means some information in which require full or partial knowledge of a direct problem. Usually direct problems determine an expected output result from given input data and inverse problems are, however, concerned with the determination of an unknown input information from some incomplete output results.

The most physics questions can be formulated as the following operator equation [10]:

$$K f = g, f \in F, g \in G$$  \hspace{1cm} (3.1)

where $K : F \rightarrow G$ is a operator form normed space $F$ to normed space $G$. The direct problem is to solve for $g$ given $K$ and $f$, but the inverse problem is to solve for $f$ given $K$ and $g$. However, there are many difficulties in solving inverse problems, which are mainly caused by the ill-posedness.

**Theorem 3.1.** The operator equation (3.1) is called well-posed if the following holds [8]:

1. **Existence:** For every $g \in G$ there is (at least one) $f \in F$ such that $K f = g$;
2. **Uniqueness:** For every $g \in G$ there is at most one $f \in F$ with $K f = g$;
3. **Stability:** The solution $f$ depends continuously on $g$; that is, for every sequence $(f_n) \subset F$ with $K f_n \rightarrow K f (n \rightarrow \infty)$, it follows that $f_n \rightarrow f (n \rightarrow \infty)$

The equation (3.1) is well-posed in the sense that the operator $K$ has a bounded inverse operator [11] while equations for which one of the above three properties does not hold are called ill-posed problem in the sense that the operator $K$ does not have a bounded inverse operator [11]. However, most of inverse problems are ill-posed. Besides, according to the spectral analysis theory of operators [12], the smoothness of kernel functions of the operator $K$ controls the degree of ill-posedness of the equation (3.1) which means that the smoother the kernel function is, the more ill-posed the equation (3.1) becomes. In addition, the degree of ill-posedness also depends on the smoothness of the exact solution which means that the unsmoother the exact solution is, the more ill-posed the equation (3.1) becomes [12].

Especially, it is difficult to solve unstable inverse problems since any small noise in the given data will cause big change to the solution. Thus, we need regularization methods to overcome ill-posedness professionally which will be introduced in the Section 4.

**Theorem 3.2.** $K$ is a linear bounded compact operator from $F$ to $G$. 

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Proof. It is easily to check that \( Kf_1 + Kf_2 = K(f_1 + f_2) \) and \( \alpha Kf = K(\alpha f) \) so the \( K : F \rightarrow G \) operator is a linear operator. For any \( f \in L^2(a, b) \), by the Cauchy inequality, we have

\[
\|Kf\|_{L^2(c,d)}^2 = \int_c^d (Kf)^2 \, dy = \int_c^d \left( \int_a^b \frac{1}{y-x} f(x) \, dx \right)^2 \, dy \leq \int_c^d \int_a^b \left( \frac{1}{y-x} \right)^2 \, dx \int_a^b f^2(x) \, dx \, dy \leq \left( \frac{1}{c-b} \right)^2 (b-a)(d-c) \|f\|_{L^2(a,b)}^2 = M\|f\|_{L^2(a,b)}^2 < +\infty,
\]

where \( M > 0 \) is a constant. Thus, from the form of the equation (3.2), we easily know \( K : F \rightarrow G \) is a bounded operator.

Since \( c > b \), the \( m \)th order derivative of \( Kf \) exists for any \( m \in \mathbb{N} \) and by the Cauchy inequality, we have

\[
\left\| \frac{\partial^m(Kf)}{\partial y^m} \right\|_{L^2(c,d)}^2 = \int_c^d \left( \int_a^b (-1)^m m! \frac{(y-x)^{m-1}}{(y-x)^m} f(x) \, dx \right)^2 \, dy \leq C\|f\|_{L^2(a,b)}^2,
\]

where \( C > 0 \) is a constant depending on \( a, b, c, d \) only. Therefore, \( Kf \in H^m(c,d) \) for any \( m \in \mathbb{N} \). Since \( m \) is arbitrary, by the embedding theorem, we know \( Kf \in C^0[c,d] \). And since \( H^k(c,d) \) is embedded into \( L^2(c,d) \) compactly, we know the operator \( K \) is a compact operator. The proof is completed.

By the above theorem 3.2, we know that the inverse problem (2.4) must be ill-posed since the compact operator must not have bounded inverse operator in infinite dimensional space [10]. Besides, due to the kernel of the integral equation is analysis, the inverse problem is severely ill-posed [12] which cause the big difficulties to invert. However, it is not enough to know the inverse problem is ill-posed so we need to figure out what type of ill-posedness the inverse problem is.

In this section, we study the ill-posedness of the inverse problem, by the theorem [], we know that the inverse problem (2.4) must be ill-posed since the compact operator must not have bounded inverse operator in infinite dimensional space [10]. Besides, due to the kernel of the integral equation is analysis, the inverse problem is severely ill-posed [12] which cause the big difficulties to invert. However, it is not enough to know the inverse problem is ill-posed so we need to figure out what type of ill-posedness the inverse problem is.

Firstly, we think the existence of the inverse problem is satisfied by default since the integral equation (2.4) have its special physical background which demand the existence must be true[ some other papers].

Secondly, we state the main result of this paper which is the rigorous proof of the uniqueness of the inverse problem (2.4).

**Theorem 3.3.** Suppose that \( f_1(x), f_2(x) \in L^2(a, b) \). If \( Kf_1 = Kf_2 = g(y) \), \( y \in [c, d] \), then we have \( f_1(x) = f_2(x) \), a. e. \( x \in [a, b] \).

Proof. Since \( K \) is a linear operator, we know that \( Kf_1 - Kf_2 = K(f_1 - f_2) = 0 \). Therefore, in order to prove \( f_1(x) = f_2(x) \), a. e. \( x \in [a, b] \), we just need to prove that \( Kf = 0 \) implies \( f(x) = 0 \), a. e. \( x \in [a, b] \).
It is easy to obtain that \( Kf = \int_a^b \frac{1}{y-x} f(x) \, dx = \int_a^b \left( \frac{1}{y} \sum_{k=0}^{\infty} \left( \frac{x}{y} \right)^k \right) f(x) \, dx \). Since \( x \in [a, b], \ y \in [c, d], \ c > b, \) we know \( \left| \frac{a}{y} \right| \leq \left| \frac{b}{c} \right| < 1, \) which implies that \( \left| \sum_{k=0}^{\infty} \left( \frac{x}{y} \right)^k \right| \leq \sum_{k=0}^{\infty} \left| \frac{b}{c} \right|^k \left| f(x) \right| \) for all \( x \in [a, b] \). Combined with \( \int_a^b f(x) \, dx < +\infty \) and the control convergence theorem, we have

\[
y \int_a^b \frac{1}{y-x} f(x) \, dx = \sum_{k=0}^{\infty} \frac{1}{y^k} \int_a^b x^k f(x) \, dx = 0, \quad y \in [c, d]. \tag{3.4}
\]

If \( d = +\infty \), by using (3.4), we have

\[
\int_a^b f(x) \, dx + \frac{1}{y} \int_a^b x f(x) \, dx + \cdots + \frac{1}{y^k} \int_a^b x^k f(x) \, dx + \cdots = 0, \quad y \in (c, +\infty). \tag{3.5}
\]

Letting \( y \to +\infty \) in (3.5), we have \( \int_a^b f(x) \, dx = 0 \). Then multiplying \( y \) on both sides of (3.5) and letting \( y \to +\infty \), we also have \( \int_a^b f(x) \, dx = 0 \). Repeating above process, we can obtain that

\[
\int_a^b x^k f(x) \, dx = 0, \quad k = 0, 1, 2, \cdots. \tag{3.6}
\]

If \( d < +\infty \), taking \( z \in D := \{ z \in \mathbb{C} : |z| \geq c \} \), we have

\[
\left| \sum_{k=0}^{\infty} \frac{1}{z^k} \int_a^b x^k f(x) \, dx \right| \leq \sum_{k=0}^{\infty} \frac{1}{z^k} \int_a^b x^k f(x) \, dx \leq \sum_{k=0}^{\infty} \frac{b^k}{c^k} \int_a^b |f(x)| \, dx < +\infty,
\]

which implies that the series \( \sum_{k=0}^{\infty} \frac{1}{z^k} \int_a^b x^k f(x) \, dx \) is convergent uniformly on \( D \). Since \( \frac{1}{z^k} \int_a^b x^k f(x) \, dx \) is analytic on \( D \) for each \( k \) and use the Weierstrass theorem, we conclude that the series \( \sum_{k=0}^{\infty} \frac{1}{z^k} \int_a^b x^k f(x) \, dx \) is analytic on \( D \). Further, we know \( \sum_{k=0}^{\infty} \frac{1}{z^k} \int_a^b x^k f(x) \, dx \) is real analytic on \( y \in (c, +\infty) \). Combined with the analytic continuation, we know that (3.4) holds for \( y > c \), i. e.

\[
\sum_{k=0}^{\infty} \frac{1}{z^k} \int_a^b x^k f(x) \, dx = 0, \quad y \in (c, +\infty).
\]

Similar to the proof process of the case \( d = +\infty \), we also conclude that \( \int_a^b x^k f(x) \, dx = 0, k = 0, 1, 2, \cdots \) for \( d < +\infty \).

Since \( C[a, b] \) is dense in \( L^2(a, b) \), then for \( f(x) \in L^2(a, b) \) and any \( \epsilon > 0 \), there exists \( \tilde{f} \in C[a, b] \), such that \( \| f - \tilde{f} \|_{L^2(a,b)} < \epsilon \). On the other hand, for \( \tilde{f} \in C[a, b] \), there exists a polynomial \( Q_n(x) \) of degree \( n \in \mathbb{N} \), such that \( \| \tilde{f} - Q_n \|_{C[a,b]} < \epsilon \) by the Weierstrass theorem. Therefore, we have

\[
\| f - Q_n \|_{L^2(a,b)} \leq \| f - \tilde{f} \|_{L^2(a,b)} + \| \tilde{f} - Q_n \|_{L^2(a,b)} \\
\leq \epsilon + \sqrt{b-a} \| \tilde{f} - Q_n \|_{C[a,b]} \\
< \epsilon + \epsilon \sqrt{b-a},
\]
By using (3.6), we know that \( \int_{a}^{b} f(x)Q_n(x)\,dx = 0 \). Combined with the Cauchy inequality, we have

\[
\|f\|_{L^2(a,b)}^2 = \int_{a}^{b} f^2(x)\,dx = \int_{a}^{b} (f^2(x) - f(x)Q_n(x))\,dx \\
\leq \int_{a}^{b} |f(x)| \cdot |f(x) - Q_n(x)|\,dx \\
\leq \left( \int_{a}^{b} f^2(x)\,dx \right)^{\frac{1}{2}} \left( \int_{a}^{b} |f(x) - Q_n(x)|^2\,dx \right)^{\frac{1}{2}} \\
= \|f\|_{L^2(a,b)} \|f - Q_n\|_{L^2(a,b)} \\
\leq (\epsilon + \epsilon \sqrt{b - a})\|f\|_{L^2(a,b)},
\]

which implies that \( \|f\|_{L^2(a,b)} \leq \epsilon + \epsilon \sqrt{b - a} \).

Letting \( \epsilon \to 0 \), we have \( \|f\|_{L^2(a,b)} = 0 \), i.e. \( f(x) = 0 \), a.e. \( x \in [a,b] \). The proof is completed. □

Thirdly, we show the instability of the inverse problem by the special case with \( a = 0, b = 1, c = 2, d = 3, f_n(x) = \sqrt{n} \cos(n \pi x), g_n(y) = \int_{0}^{1} \frac{1}{y-x} f_n(x)\,dx \). For the special case, we have \( \|f_n\|_{L^2(0,1)} \to \infty \) and \( \|Kf_n\|_{L^2(2,3)} = \frac{1}{\sqrt{n\pi}} (\int_{\frac{1}{y-x}}^{1} (\int_{0}^{1} \frac{1}{y-x} \sin(n \pi x) dx)^2 dy)^{1/2} \leq \frac{1}{\sqrt{n\pi}} \to 0, n \to \infty \), which means \( f_n \) fails in depending continuously on the given data \( g_n \).

In conclusion, the inverse problem (2.4) satisfies the existence, uniqueness and instability. Facing the severely ill-posedness and instability, classical methods are out of work and regularization methods need to be used to solve it professionally.

## 4 Regularization Methods

### 4.1 Introduction to the Regularization Theory

As we all know, it is difficult to directly solve problems in infinite dimensional space to get analysis solution so we must turn them into finite dimensional space to get numerical solution [13]. At the same time, due to the ill-posedness of inverse problems, we have to use regularization methods to overcome the ill-posedness [7]. According to the different sequence of the two steps: discretization and regularization, the regularization methods for solving ill-posed inverse problems in infinite dimensional space can be divided into the following two categories [8]:

**A1:** Firstly, the regularization methods for ill-posed problems in infinite dimensional space are used to obtain the approximate well-posed problems in finite dimensional space. Secondly, suitable numerical methods are used to solve the well-posed problems and get the numerical solutions in finite dimensional space.
A2: Firstly, the ill-posed problems on infinite dimensional space are discretized to obtain the approximate problems in finite dimensional space which are still ill-posed problems. Secondly, regularization methods are used to overcome the ill-posedness of problems in finite dimensional space.

There are popular regularization methods belonging to A1, such as Tikhonov regularization method [14], Lanweber iteration regularization [15], non-stationary iterative Tikhonov regularization method [16], iterative ensemble Kalman method [17] and alternating direction method of multipliers [18]. For A2, there are Galerkin methods [20], Collocation methods and etc [19]. The regularization methods belonging to A2 are always called the self-regularization or the regularization by projection since if the dimensions of discrete space is properly selected and the discrete method is effective, the regularization effect will be produced automatically for ill-posed problems and no additional techniques are needed [21]. However, in this paper, the discussion about A2 will be talked in the future and we only adopt the A1.

Since the data is usually obtained by measurement and unavoidably contains noise, instead of the exact data \( g \), we only have the noisy data \( g^\delta \) satisfying \( \|g^\delta - g\|_Y \leq \delta \) for the noise level \( \delta > 0 \). Thus, our aim is to solve the following perturbed integral equation.

\[
K f^\delta = \int_a^b f^\delta(x) \frac{y-x}{y-x} dx = g^\delta(y), \quad y \in [c, d]
\] (4.1)

Due to the instability of the inverse problem, a little noise in \( g(y) \) will make a significant difference to inversion result \( f(x) \). Therefore, the best we hope is to determine an approximate solution \( f^\delta(x) \) near with the exact solution \( f(x) \) and approximate solution \( f^\delta(x) \) depends continuously on the data \( g^\delta(x) \). By using regularization methods, the hope can be achieved effectively. It is easy to get the mathematical idea of regularization methods which is to construct a suitable bounded approximate operator \( R : G \to F \) of the unbounded inverse operator \( K^{-1} : \mathcal{R}(K) \to F \) [8].

The definition of the regularization operator is as follow.

**Theorem 4.1.** A regularization strategy is a family of linear and bounded operators \( R_\alpha : G \to F, \alpha > 0 \), such that \( \lim_{\alpha \to 0} R_\alpha K f = f \) for all \( f \in F \), where the \( \alpha \) is the regularization parameter [8].

Form the above definition, it can be seen that for exact data, the \( R_\alpha g \) converges to \( f \) for the exact solution \( f \) as \( \alpha \to 0 \). Besides, form the above definition and the compactness of \( K \), we conclude the following theorem.

**Theorem 4.2.** Let \( R_\alpha \) be a regularization strategy for a compact operator \( K : F \to G \) where dim\( F = \infty \). Then we have [8]

1. The operator \( R_\alpha \) are not uniformly bounded; that is, there exists a sequence (\( \alpha_j \)) with \( \|R_{\alpha_j}\| \to \infty \) for \( j \to \infty \).
The sequence \((R_\alpha K x)\) does not converge uniformly in bounded subsets of \(X\); that is, there is no convergence \(R_\alpha K\) to the identity \(I\) in the operator norm.

In practice, we must consider the case where the data has noise. Let \(g \in \mathcal{R}(K)\) be the exact right-hand side and \(g^\delta \in G\) be the noise data with \(\|g - g^\delta\|_2 \leq \delta\) and define \(f^\delta_\alpha = R_\alpha g^\delta\) as an approximate solution of \(K f = g\). Then the total error between the approximate solution \(f^\delta_\alpha(x)\) and the exact solution \(f(x)\) is split into two parts by the triangle inequality:

\[
\|f^\delta_\alpha - f\|_F \leq \|R_\alpha g^\delta - R_\alpha g\|_F + \|R_\alpha g - f\|_F \\
\leq \|R_\alpha\| \|g^\delta - g\|_G + \|R_\alpha K f - f\|_F \\
\leq \delta \|R_\alpha\| + \|R_\alpha K f - f\|_F
\]

According to the theorem 4.2, the term \(\|R_\alpha\|\) tends to infinity as \(\alpha \to 0\) while the term \(\|R_\alpha K f - f\|_F\) tends to zero as \(\alpha \to 0\). Thus, the regularization parameter \(\alpha\) should be chosen carefully strictly to keep the total error as small as possible. Luckily, there are many popular ways to select the regularization parameter \(\alpha\) which will be discussed in Section 4.4 in detail.

### 4.2 Tikhonov Regularization

The Tikhonov regularization method has been widely used to solve linear ill-posed inverse problems [14] [22]. However, the Tikhonov regularization method has the tendency to over-smooth solutions and hence are not quite successful to capture special features such as sparse solutions and discontinuous solutions [7]. For these special solutions, it can be inverted well by the methods [23] [18] [24]. In this study, the Tikhonov regularization method is used to solve the ill-posed inverse problem adequately. The basic idea is to use the minimizer of the following variational problem to approach the exact solution [8], i.e., solving

\[
f^\delta_\alpha = \arg \min_{f \in L^2(a,b)} J(f) = \frac{1}{2} \|K f - g^\delta\|_{L^2(c,d)}^2 + \frac{\alpha}{2} \|f\|_{L^2(a,b)}^2,
\]

where \(\alpha > 0\) is called a regularization parameter and the minimizer \(f^\delta_\alpha\) is called a regularized solution of problem (2.4). Besides, the minimizer \(f^\delta_\alpha\) satisfies the following operator equation:

\[
\alpha f^\delta_\alpha + K^* K f^\delta_\alpha = K^* g^\delta
\]

where the \(K^*\) is the adjoint operator of \(K\) given by \(K^* g = \int_c^d \frac{1}{y-x} g(y) dy, x \in [a, b]\). Thus, the solution \(f^\delta_\alpha\) of equation (4.4) can be written in the form [8] \(f^\delta_\alpha = R_\alpha g^\delta\) with

\[
R_\alpha := (\alpha I + K^* K)^{-1} K^* : G \to F
\]

The operator \(R_\alpha\) is a regularization strategy met the theorem (4.1)[see].
By the above Tikhonov regularization theory and the suitable regularization parameter, it can be got that the regularized solution \( f_\alpha^\delta \) converges to the exact solution \( f \) [8], i.e., we have

\[
\|f_\alpha^\delta - f\|_{L^2(a,b)} \rightarrow 0, \text{ as } \delta \rightarrow 0. \tag{4.6}
\]

As can be seen from the equation (4.6), when the condition that we use the regularization theory and get suitable regularization parameter and the noise \( \delta \rightarrow 0 \) is satisfied, the regularized solution must converges to the exact solution. Thus, the inverse problem approach of non-perturbation QCD is a first principle approach.

### 4.3 Numerical Method of Tikhonov Regularization Method

After using Tikhonov regularization method to overcome the ill-posedness of the inverse problem (2.4), we need to use a suitable numerical method to get the numerical solution. Thus, in this section, the finite dimensional approximation method is used to solve the variational problem (4.3). Other discrete methods may be suitable and will be discussed in the future.

We discrete the interval \([a, b]\) by grid points \( x_i = a + ih, \ i = 0, 1, 2, \cdots, n \) where the step size is \( h = \frac{b-a}{n} \) and use piecewise linear basis functions, i.e. take the basis functions as the following hat functions for \( i = 1, 2 \cdots, n - 1 \)

\[
\varphi_i(x) = \begin{cases} \frac{x-x_i}{h}, x \in [x_{i-1}, x_i], \\ -\frac{x-x_{i+1}}{h}, x \in [x_i, x_{i+1}], \\ 0, \text{otherwise}, \end{cases}
\]

\[
\varphi_0(x) = \begin{cases} -\frac{x-x_{i+1}}{h}, x \in [x_0, x_1], \\ 0, \text{otherwise}, \end{cases}
\]

and

\[
\varphi_n(x) = \begin{cases} \frac{x-x_{n-1}}{h}, x \in [x_{n-1}, x_n], \\ 0, \text{otherwise}. \end{cases}
\]

Taking a finite dimensional subspace of \( L^2(a, b) \) denoted by \( X_n = \text{span}\{\varphi_0, \varphi_1, \cdots, \varphi_n\} \), we solve the following minimization problem in the subspace \( X_n \)

\[
f_{\alpha,n}^\delta = \arg \min_{f \in X_n} J(f) = \frac{1}{2} ||Kf - g^\delta||_{L^2(c,d)}^2 + \frac{\alpha}{2} ||f||_{L^2(a,b)}^2. \tag{4.7}
\]

Suppose the minimizer is \( f_{\alpha,n}^\delta(x) = \sum_{i=0}^{n} c_i \varphi_i(x) \) and put it into the functional \( J(f) \) in (4.7), then we have

\[
J(f_{\alpha,n}^\delta) = \frac{1}{2} \left\| \sum_{i=0}^{n} c_i (K\varphi_i - g^\delta) \right\|_{L^2(c,d)}^2 + \frac{\alpha}{2} \left\| \sum_{i=0}^{n} c_i \varphi_i \right\|_{L^2(a,b)}^2
\]

\[
= \frac{1}{2} \sum_{i,j=0}^{n} c_i c_j (K\varphi_i, K\varphi_j)_{L^2(c,d)} - \sum_{i=0}^{n} c_i (K\varphi_i, g^\delta)_{L^2(c,d)} + \frac{1}{2} \|g^\delta\|_{L^2(c,d)}^2 + \frac{\alpha}{2} \sum_{i,j=0}^{n} c_i c_j (\varphi_i, \varphi_j)_{L^2(a,b)}. \]
Let the derivative of the above functional $J(f_{a,n}^\delta)$ to $c_i$ be zero for $i = 0, 1, \cdots, n$, then we know that the unknown coefficients in the minimizer $f_{a,n}^\delta(x)$ satisfy the following linear system of algebra equations

$$(A + \alpha B)C = D,$$

(4.8)

where the $(i, j)$ element of matrix $A$ is given by $A_{ij} = (K\varphi_i, K\varphi_j)_{L^2(a,b)}$ and the $(i, j)$ element of matrix $B$ is given by $B_{ij} = (\varphi_i, \varphi_j)_{L^2(a,b)}$ and the $i$th element in the right hand side vector is given by $D_i = (K\varphi_i, g^\delta)_{L^2(a,b)}$ and the unknown vector $C = (c_0, c_1, \cdots, c_n)^T$. Solving the linear system (4.8) to obtain the solution $C$, we get the minimizer $f_{a,n}^\delta(x) = \sum_{i=0}^n c_i \varphi_i(x)$.

In addition, we proof the following theorem 4.3 to find that the numerical solutions $f_{a,n}^\delta$ converge to the analysis solutions $f_a^\delta$ as discretization step $n \to \infty$.

**Theorem 4.3.** If the noise $\delta$ and the regularization parameter $\alpha$ are fixed, we have $\| f_{a,n}^\delta - f_a^\delta \|_{L^2(a,b)} \to 0$, as $n \to \infty$.

**Proof.** Let $P_n : L^2(a,b) \to X_n$ be the orthogonal project operator, i.e. for $u \in L^2(a,b)$, so we have $(u - P_n u, v)_{L^2(a,b)} = 0$ for all $v \in X_n$. From the finite element theory, we know $\| u - P_n u \|_{L^2(a,b)} \to 0$, as $n \to \infty$, for any $u \in H^1(a,b)$.

Since $J(f_a^\delta) \leq J(f_{a,n}^\delta) \leq J(P_n f_a^\delta)$, we have

$$0 \leq J(P_n f_a^\delta) - J(f_a^\delta) = \frac{1}{2} \| (P_n f_a^\delta - f_a^\delta) \|_{L^2(a,b)}^2 + (K(P_n f_a^\delta - f_a^\delta), K f_a^\delta - g^\delta)_{L^2(a,b)}$$

$$+ \frac{\alpha}{2} \| P_n f_a^\delta - f_a^\delta \|_{L^2(a,b)}^2 + \alpha (P_n f_a^\delta - f_a^\delta, f_a^\delta)_{L^2(a,b)}$$

$$\leq \frac{1}{2} \| K \|^2 \| P_n f_a^\delta - f_a^\delta \|_{L^2(a,b)}^2 + \| K \| \| P_n f_a^\delta - f_a^\delta \|_{L^2(a,b)} \| K f_a^\delta - g^\delta \|_{L^2(a,b)}$$

$$+ \frac{\alpha}{2} \| P_n f_a^\delta - f_a^\delta \|_{L^2(a,b)}^2 + \alpha \| P_n f_a^\delta - f_a^\delta \|_{L^2(a,b)} \| f_a^\delta \|_{L^2(a,b)}^2.$$

The minimizer $f_a^\delta$ of the variational problem (4.3) satisfies the following operator equation $\alpha f_a^\delta + K^* K f_a^\delta = K^* g^\delta$. Note that the range of the operator $K^*$ is in $C^\infty[a,b]$, thus $f_a^\delta \in H^1(a,b)$. Therefore $\| f_a^\delta - P_n f_a^\delta \|_{L^2(a,b)} \to 0$ as $n \to \infty$. From estimate (4.9), we have $J(P_n f_a^\delta) - J(f_a^\delta) \to 0$, as $h \to \infty$. Thus, we have $J(f_{a,n}^\delta) \to J(f_a^\delta)$ as $h \to 0$ which means $f_{a,n}^\delta$ is a minimizer sequence. It deduces $\| f_{a,n}^\delta \|_{L^2(a,b)}$ is bounded by a constant independent of $n$, thus there is a subsequence $f_{a,h_n}^\delta$ satisfying

$$f_{a,h_n}^\delta \to v, \text{ weakly in } L^2(a,b), \text{ as } k \to \infty.$$

Since $K$ is a linear bounded operator, we have $K f_{a,n}^\delta \to K v$, weakly in $L^2(a,b)$, as $k \to \infty$. By the sequentially weakly lower semi-continuity of $L^2$-norm, we have

$$J(v) \leq \liminf_{k \to \infty} J(f_{a,n}^\delta) = J(f_a^\delta).$$
That indicates \( v \) is the minimizer of \( J \) over \( L^2(a, b) \). It is well-known that the minimizer is unique \([\cdot]\) so we have \( v = f^\delta_a \). Further, we have \( f^\delta_{a, n_k} \rightarrow f^\delta_a \) as \( k \rightarrow \infty \).

If \( \lim \sup_{k \rightarrow \infty} \| f^\delta_{a, n_k} \|_{L^2(a, b)} > \| f^\delta_a \|_{L^2(a, b)} \), there exits a subsequence also denoted as \( f^\delta_{a, n_k} \) such that \( \lim_{k \rightarrow \infty} \| f^\delta_{a, n_k} \|_{L^2(a, b)} > \| f^\delta_a \|_{L^2(a, b)} \). Then by the sequentially weakly lower semi-continuity of \( L^2 \)-norm, we have

\[
\frac{1}{2} \| K f^\delta_a - g^\delta \|_{L^2(c, d)} \leq \lim \inf_{k \rightarrow \infty} \frac{1}{2} \| K f^\delta_{a, n_k} - g^\delta \|_{L^2(c, d)} \leq \lim \sup_{k \rightarrow \infty} \frac{1}{2} \| K f^\delta_{a, n_k} - g^\delta \|_{L^2(c, d)}
\]

\[
= \lim \sup_{k \rightarrow \infty} \left( J(f^\delta_{a, n_k}) - \frac{\alpha}{2} \| f^\delta_{a, n_k} \|_{L^2(a, b)} \right) < J(f^\delta_a) - \frac{\alpha}{2} \| f^\delta_a \|_{L^2(a, b)} = \frac{1}{2} \| K f^\delta_a - g^\delta \|_{L^2(c, d)}
\]

which is impossible undoubtedly. Therefore we have

\[
\| f^\delta_{a, n_k} \|_{L^2(a, b)} \leq \lim \inf_{k \rightarrow \infty} \| f^\delta_{a, n_k} \|_{L^2(a, b)} \leq \lim \sup_{k \rightarrow \infty} \| f^\delta_{a, n_k} \|_{L^2(a, b)} \leq \| f^\delta_a \|_{L^2(a, b)}
\]

further we have \( \| f^\delta_{a, n_k} \|_{L^2(a, b)} \rightarrow \| f^\delta_a \|_{L^2(a, b)} \) as \( k \rightarrow \infty \). Combined with \( f^\delta_{a, n_k} \rightarrow f^\delta_a \) as \( k \rightarrow \infty \) and the minimizer \( f^\delta_a \) is unique, the convergence result is satisfied. The proof is completed. \( \square \)

### 4.4 Selection Rules of the Regularization Parameter

This section is devoted to introduce the way to select regularization parameter \( \alpha \). Just like the previous theoretical analysis in section 4.2, regularization parameter \( \alpha \) should be admissible to get the total smallest and obtain a good approximate solution. There are two kinds of ways to select regularization parameter: priori choice rule and posteriori choice rule.

**B1:** The prior choice rules are based on the smoothness conditions of the exact solution, however, which are actually difficult to get in advance \([8]\) \([7]\) \([9]\). The prior selection method based on Tikhonov regularization method can be seen in the following theorem \([8]\).

**Theorem 4.4.** For Tikhonov regularization method, if we let \( f = K^* z \in \mathcal{R}(K^*) \) with \( \| z \| \leq E \). We choose \( \alpha = c \delta / E \) for some \( c > 0 \). Then the following estimate holds:

\[
\| f^\delta_a - f \|_X \leq \frac{1}{2} (1/ \sqrt{c} + \sqrt{c}) \sqrt{\delta E} \quad (4.10)
\]

Let \( f = K^* K z \in \mathcal{R}(K^* K) \) with \( \| z \| \leq E \). The choice \( \alpha = c (\delta / E)^{2/3} \) for some \( c > 0 \) leads to the error estimate

\[
\| f^\delta_a - f \|_X \leq \left( \frac{1}{2 \sqrt{2}} + c \right) E^{1/3} \delta^{2/3} \quad (4.11)
\]

It can be seen that the priori condition \( x = K^* z \in \mathcal{R}(K^*) \) or \( x = K^* K z \in \mathcal{R}(K^* K) \) is hard to meet in the above theorem. Thus, the priori choice rules are rarely used which the posteriori choice rules are usually used when selecting the regularization parameter \( \alpha \).
B2: The posterior choice rules are based on the noise data $g^\delta(y)$ or noise data $g^\delta(y)$ and noise level $\delta$ [8] [7] [9]. There are many popular posteriori choice rule such as Morozov’s discrepancy principle [25], L-curve method [26], generalized discrepancy principle [27].

In this study, we use the L-curve method to obtain the regularization parameter $\alpha$. Other methods will be discussed in the future and it is enough and good to solve the inverse problem (2.4). The L-curve method is to use the minimizer of the following function to get the admissible regularization parameter.

$$\alpha = \arg \min_{f^\delta \in L^2(a,b)} \phi(\alpha) = \|f^\delta\|_F \|g^\delta - Kf^\delta\|_G$$

(4.12)

It is easy to know the basic idea of the L-curve method which is to minimize both the residual term $\|Kf^\delta - g^\delta\|_G$ and the regularization term $\|f^\delta\|_F$.

It is efficient to use the same discrete method as in the section 4.3 to discrete the variational problem (4.12) to get proper regularization parameter $\alpha$.

In a short summary, the ill-posed inverse problem can be solved by two steps in practice: choose one regularization method and select the proper value of the regularization parameter.

5 Toy Models

The basics of the inverse problem approach to calculate the non-perturbative quantities are introduced in the above sections. Its mathematical properties and how to do the calculations are all well explained. To vividly show the inverse problem and how it works, we will test some toy models and discuss in details about this novel method.

The purpose of this work is to propose the inverse problem approach and manifest that it is valid for the calculation on the non-perturbative QCD quantities. As a beginning work, we use the Tikhonov regularization method and the L-curve method to get regularization parameter, which are simple in mathematics and in practice and thus are very helpful to develop the new approach in the future. Several other regularization methods will be left for further studies in the future.

Without a regularization, the solutions of the inverse problem are unstable and thus of large uncertainties. One of the most important issue is to test what the precision of solutions might be in this approach with a regularization. This is also important for the predictions on the non-perturbative quantities in the practical problems of particle physics. Basically, we will test two kinds of effects of parameters. One is the parameters in the method itself, including the regularization parameter $\alpha$ and the separation scale $\Lambda$. The other one is the input parameters in the right-handed side of the Eq.(??). In order to see the theoretical uncertainties clearly, we will test the input uncertainties as a linear type. Taking the linear combination of uncertainties as an example, $f(x) = a_1f_1(x) + a_2f_2(x)$, so then
The influence of the regularization method and regularization parameter on the solutions are discussed in Figs. 2-4 for each model, respectively. It can be seen that some values of the regularization parameters $\alpha$ taken as the values of regularization methods. This confirms what we discussed in the previous sections.

It can be clearly seen in Fig. 1 that the solutions obtained by this direct way are very unstable and far away from the true values. Therefore, the ill-posed inverse problem can not be well solved without any regularization for each toy model. Some typical functions are chosen as the toy models, which are either helpful to clarify the properties of inverse problems or close to the real physical problems. Three kind of functions are chosen as: monotonic functions, simple non-monotonic functions, and low oscillation functions.

Model 1: a monotonic function as $f_1(x) = \sin(\pi x)$, $f_2(x) = e^x$;

Model 2: a simple non-monotonic function as $f_1(x) = xe^{-x}$, $f_2(x) = 0$;

Model 3: an oscillating function as $f_1(x) = \sin(2\pi x)$, $f_2(x) = x$.

Since the origin integral equation in Eq. (??) is split into two parts of perturbative and non-perturbative contributions, the continuity of the imaginary part of correlation function is actually a boundary condition of the inverse problem. The more we know, the better the inversions will be. Thus, the boundary conditions of $f(x)$ should be utilized to get better inversion results in all toy models.

Taking the boundary conditions as $f(0) = M$, $f(b) = N$, the function $f(x)$ can be written as $f(x) = u(x) + v(x)$, where $v(x)$ is linear and satisfying the same boundary conditions as $f(x)$, $v(x) = M(\frac{x-b}{b-0}) + N(\frac{x-0}{b-0})$. Then the unknown function $u(x)$ can be solved by the following integral equation,

$$\int_a^b \frac{u(x)}{y-x} dx = g^\delta - \int_a^b \frac{v(x)}{y-x} dx := G^\delta$$

with $u(a) = u(b) = 0$. Using the Tikhonov regularization method and the L-curve method to solve $u^\delta_a$, the solution can be obtained as $f^\delta_a(x) = u^\delta_a(x) + v(x)$. Similarly, if the values of some other points in $f(x)$ are known accurately, we can also use them to improve the inversion result.

5.1 Importance of regularization methods and regulators

The influence of the regularization method and regularization parameter on the solutions are discussed in this subsection.

At the beginning, we directly solve the inverse problem without any regularization for each toy model. It can be clearly seen in Fig. 1 that the solutions obtained by this direct way are very unstable and far away from the true values. Therefore, the ill-posed inverse problem can not be well solved without any regularization methods. This confirms what we discussed in the previous sections.

Then we test the influence of the Tikhonov regularization method. The regularization parameter are taken as the values of $\alpha = 10^{-i}$, $i = 1, 2, \cdots, 20$. The solutions are obtained for each value of $\alpha$, shown in Figs. 2-4 for each model, respectively. It can be seen that some values of the regularization parameters
Figure 1: The solutions without any regularization method. The figures from the left to the right correspond to the toy models 1, 2 and 3, respectively. It can be clearly seen that the solutions are unstable without any regularization.

Figure 2: The solutions of Model 1 by the Tikhonov regularization method with the regularization parameter $\alpha = 10^{-i}, i = 1, 2, \cdots, 20$, written on the top of each figure. The blue curves are the true solution, while the red curves are the solutions corresponding to each value of the regularization parameter. It can be found that some values of the regularization parameter can be helpful to get a good result.

can be helpful to get a good result. So the regularization methods are necessary to solve the ill-posed inverse problems. Besides, the inverse problem of the dispersion relations can be solved as seen in this way.

The unstable results in the case of small values of $\alpha$ can be easily understood that such small $\alpha$ can not behave as a real regularization, similarly to the case without any regularization method. The results with large $\alpha$ is not good as well, because the penalty term dominates over the original problem. Therefore,
Figure 3: Same as Fig.2 but for Model 2.

Figure 4: Same as Fig.2 but for Model 3.
the value of the regularization parameter can be neither too small nor too large.

This does not mean the results are sensitive to the value of $\alpha$. From Figs. 2-4, it can be seen that there are still large room for the value of $\alpha$, ranging by several orders of magnitude, to provide a good results. This feature can also be seen in the following subsection.

Comparing the results among Figs. 2, 3 and 4, it can be found that the ranges of $\alpha$ allowed for the good results are larger for the monotonic functions, but smaller for the oscillating functions. This can be understood that the Tikhonov regularization in the $L^2$ space flatten the oscillating functions. Therefore, the more smooth the functions are, the better the solutions given by the Tikhonov regularization are. Of course, some other regularization methods would work for the case of oscillating or non-smooth functions. But we leave such studies in the future, and focus on the Tikhonov regularization in this work.

5.2 Impact of uncertainties of inputs

In the physical world, it is unable to avoid the uncertainties of any data. The solutions of the inverse problems are significantly affected by the noises of the input data. In our inverse problem of dispersion relation with the proved property of unstable solutions, one of the key issue is to control the uncertainties of solutions by the regularization method. Besides, as proved in the previous section, the solutions should approach to the true values as the input error vanishing with a suitable regularization method. We will test all of these features here.

The errors of input parameters are tested at the level of 30%, 10% and 1%, respectively. The results are shown in Fig. 5, with the input errors of 30%, 10% and 1% from the left to the right, and the models 1, 2 and 3 from the top to the bottom, respectively. The uncertainties of the solutions are almost at the same level of the input errors. The smaller the input errors are, the more precise the solutions are. This is consistent with the expectation of the regularization method as we discussed before.

This indicates a very important feature of the inverse problem approach that the uncertainties of the predictions strongly depend on the input errors. If the regularization method is suitably used, the prediction of the predictions can be systematically improved by lowering down the input errors. It will be found in the following subsection that the problem of the slightly inconsistency with the true solutions for the 1% input errors would be solved by the improved regularization method.

5.3 Improved Regularization Method

In the spirit of the inverse problem, the more we know, the better the solutions would be. A priori condition can be included to improve the regularization method. In our toy models, if we know the solutions are smooth functions, the norm space can be changed to be a better one. In the previous studies,
Figure 5: Impact of errors of inputs. The input errors are 30%, 10% and 1% from the left to the right, with the models 1, 2 and 3 from the top to the bottom. The uncertainties of the solutions are almost at the same level of the input errors.

we only use the $L^2$ space which is include much larger situations. But if the smoothness of the solutions is know, we can use a smaller space, the $H^1$ space, whose norm is defined as $\|f\|_{H^1(a,b)} = \int_a^b (f^2 + f'^2) dx$ where $f'$ is the derivative of $f$. It is obviously that the $H^1$ space is smooth and derivable. Since if $f(x) \in H^1$, $f(x) \in L^2$, the mathematical properties of the inverse problem (2.4) after changing the space $X$ are still the same: the solution of the inverse problem is still exist, unique and unstable. This approach is equivalent to limit the exact solution to a small subspace to obtain a better inversion solution. What we should do is only to change the norm from $L^2$ to $H^1$ in the Tikhonov regularization method and the L-curve method.

The results are shown in Fig.6. It can be clearly seen that the solutions are significantly improved compared to the ones in Fig. 5. Especially, the model 3 can be solved in some sense, which can never be done before. In the following of this paper, we will use the $H^1$ space to show the results.

Therefore, the solutions can be better solved by improving the regularization method.
Figure 6: Impact of the improvement of the regularization method, with the $L^2$ space of $f(x)$ changed to be the $H^1$ space. The input errors are 30%, 10% and 1% from the left to the right, with the models 1, 2 and 3 from the top to the bottom. The solutions are significantly improved compared to the results in Fig. 5.

5.4 Insensitivity of the regularization parameter and the separation scale

In general, there are only two free parameters in the inverse problem, the regularization parameter $\alpha$ and the separation scale $\Lambda$, except for the input parameters. It is necessary to test whether the solutions are sensitive to these two parameters or not. We vary values of $\alpha$ and $\Lambda$ to test whether there exist a plateau for each of them. A plateau indicates that the results are insensitive to the values of the parameters.

We firstly vary the values of $\alpha = 10^{-i}, i = 1, 2, \cdots, 20$, to find the corresponding solutions, and then calculate the norm of $\|f^{\delta}_i - f\|_{H^1}$ which measure the goodness of the solutions. The input data are artificially given by an error of 10%. The results are shown in Fig. 7. It can be found that there exist plateaus for model 1 and 2, which indicates that the solutions are not sensitive to the values of $\alpha$ for these two models. We have also tested that the results in the plateaus are perfectly consistent with the true values, whose figures are not shown to make the paper more convenient to read. This makes the inverse problem approach very suitable for some non-perturbative calculations. The plateau is not very clear for
model 3, since the Tikhonov regularization method is not very suitable the oscillating functions.

Figure 7: The norm of $\|f_\delta^\alpha - f\|_{H^1}$ with the variation of $\alpha = 10^{-i}, i = 1, 2, \cdots, 20$. The red points are the values of the L-curve method. A very clear plateau can be seen for model 1 and 2, which indicates that the solutions are not sensitive to the regularization parameter.

Similarly, we test the insensitivity of the solutions to the separation scale $\Lambda$, shown in Fig. 8, with $\Lambda$ ranging from 2 to 8. It is clearly seen that a plateau exists in model 1 and 2. We have also tested that the results in the plateaus are good enough. So the solutions are not sensitive to the values of the separation scale. This can be understood that the $\Lambda$ is not a very clear scale to separate the perturbative and non-perturbative range. The continuous condition at $\Lambda$ might be even more helpful to make the inverse problem approach not sensitive to the value of $\Lambda$. The solutions of model 3 depend on $\Lambda$ since there are more oscillations with larger $\Lambda$.

Figure 8: The values of $f_\delta^\alpha$ with the variation of $\Lambda$ ranging from 2 to 8. A very clear plateau can be seen for model 1 and 2, which indicates that the solutions are not sensitive to the separation scale $\Lambda$.

We have also tested the impact of some quantities in the numerical calculations. The range of $s$ in Eq.(2.3) can be artificially chosen, say $s \in [c,d]$. In principle, $c$ should be close to $\Lambda$, while $d$ should be as large as infinity. In the practice, both of them have to be taken as two fixed values in our numerical computations. We found that perfect plateaus exist for $c$ in the range close to $\Lambda$ and for $d$ in the range of large enough, which are however not shown explicitly since this behavior can be naively expected and easily understood.

In conclusion, the solutions of monotonic and simple non-monotonic functions are not sensitive to the values of the regularization parameter and the separation scale. Therefore, the inverse problem works
well for such kinds of problems, with the uncertainties well controlled from the method itself.

6 Summary

In this work, we well develop the theoretical framework of the inverse problem approach, with the strict mathematical theorems and proofs. It starts from the dispersion relation of quantum field theory, separating the high-energy and low-energy scales and using the known perturbative theories to solve the unknown non-perturbative quantities by the inverse problem. We prove that the inverse problem of dispersion relation is ill-posed, with unique but unstable solutions. The regularization methods must be used to get the stable approximate solutions. The method is based on the strict mathematics, without any artificial assumptions. We have test some toy models to vividly show the main features of the inverse problem. It can be found that this approach can systematically improve the precision of the solutions.

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