ON THE PROBLEM OF THE BOUND STATES IN
THE FRAMEWORK OF THE PADE APPROXIMANTS

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ABSTRACT

It is suggested that the dependence of the poles of the Padé approximants on the masses of the external virtual particles for an off-mass-shell scattering amplitude may be used in order to improve, by means of a variational principle, the determination of the bound states.

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1. The technique of Padé approximants constructed from the perturbative expansion of the S matrix has been recently proposed ¹⁾ in order to investigate the problem of bound states (or resonances, or Regge poles) in relativistic field theories.

It is the aim of this note to point out an ambiguity in the method of Padé approximants, namely an unwanted dependence of the position of the bound states on some "external" parameters, and to suggest the use of this extra dependence in order to improve the approximation. The external parameters will be considered as free parameters in the ansatz of a variational principle, from which the best choice can be obtained.

We briefly recall the method of the Padé approximants. One starts by writing the perturbative expansion of the scattering amplitude (let us call it T) for a scattering process, say $\pi\pi$ scattering, calling λ the coupling constant

$$T = \lambda t_1 + \lambda^2 t_2 + \dots \quad (1)$$

The diagonal Padé approximant of order N , P^N , is defined as the ratio of two polynomials of order N in λ such that its series expansion reproduces the expansion (1) up to the order λ^{2N} included. It has been shown ²⁾ that the result can be written in the form

$$P^N = \lambda m^T M^{-1} m \quad (2)$$

where M is the $N \times N$ matrix

$$M_{ij} = t_{i+j-1} - \lambda t_{i+j} \quad i, j = 1, \dots, N \quad (3)$$

and m is the column vector

$$m_i = t_i \quad (4)$$

The matrix elements appearing in the calculation are usually taken to be matrix elements in partial waves, i.e., between eigenstates of the angular momentum. The assumption is that $\lim_{N \rightarrow \infty} P^N = T$. P^N is then regarded to be an approximation for T , also for small N , i.e., $N=1$ or 2 . The approximated bound states or resonances are found by looking at the poles of P^N in the complex energy plane. Hence, the approximate position of the poles is given by the equation

$$\det M = 0 \quad (5)$$

The aforementioned ambiguity appears when one considers off-mass shell amplitudes as well as on-mass shell ones. Let us take for instance the photo-production via virtual photons, i.e., the electroproduction to the lowest order in the e.m. coupling constant. We can write the series expansion in the strong coupling constant Λ , apply the Padé method and look for the poles. The position of the poles will depend however on the virtual mass of the photon.

The same will happen when the four-point Green function, relevant for the process of interest, is considered. The Padé approximant can be constructed and the position of the bound states given by Eq. (5) will depend on the masses of the external virtual particles. One can ask therefore for the "best" choice of the external masses, and it is proposed here to give a meaning to the best choice by means of the use of a variational principle.

2. It is well known ^{1),2)} that P^N correspond to the approximate solution of the Lippmann-Schwinger ³⁾ variational principle. In potential theory the principle states that the scattering amplitude $\langle f|T|i \rangle$ is determined by finding the stationary value of

$$\langle f|T|i \rangle = \frac{\langle f|V| \psi^+ \rangle \langle \psi^- | V | i \rangle}{\langle \psi^- | V | \psi^+ \rangle - \langle \psi^- | V \frac{1}{E_0 + i\epsilon - H_0} V | \psi^+ \rangle} \quad (6)$$

where V is the interaction and H_0 the free Hamiltonian, E is the total energy, i.e., for physical processes the energy of $|i\rangle$ and $|f\rangle$.

If $|i\rangle$ is (in our example) a two-pion state of angular momentum J $|\pi\pi Jk\rangle$ ($k = \sqrt{E}$) a particular ansatz [due to Cini and Fubini ⁴] is the following

$$|\psi^+\rangle = \sum_{n=1}^N a_n \left(\frac{1}{E + i\varepsilon - H_0} V \right)^{n-1} |\pi\pi Jk\rangle \quad (7)$$

and the same for $|\psi^-\rangle$ apart from changing $\varepsilon \rightarrow -\varepsilon$. The variation over a_i gives the solution (2), i.e., it is P^N .

There is however a variational principle which can be directly applied in order to find bound states, and which is closely related to (6). The principle is best stated in terms of the eigenvalues of the coupling constant λ ($V = \lambda \psi$), i.e., the values of λ for which at a given energy a bound state or a resonance appears. The eigenvalues of λ are stationary values for the expression

$$\frac{1}{\lambda} = \frac{\langle \psi | \psi \frac{1}{E - H_0} \psi | \psi \rangle}{\langle \psi | \psi | \psi \rangle} \quad (8)$$

[$\varepsilon = 0$ for a bound state. In general we take E to be complex. For resonance actually $\langle \psi |$ is not the h.c. of $|\psi\rangle$, but rather the h.c. of $|\psi(E^*)\rangle$.]

If we choose for $|\psi\rangle$ the ansatz (7) we obtain the homogeneous system of equations for the a_i 's

$$M_{ij} a_j = 0 \quad (9)$$

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where M_{ij} is given by (3). The eigenvalues are thus given by Eq. (5). It is seen that in general the values of λ given by the stationary value of (8) are singularities for the solution of the variational principle stated in (6).

Expression (8) depends only on the values of $|\psi\rangle$ in the region in which the potential ψ is different from zero. $|\psi\rangle$ may even be a non-normalizable state, provided that the matrix elements appearing in (8) have a meaning. Indeed the related variational principle gives rise to the homogeneous equation for $\psi|\psi\rangle$ rather than for $|\psi\rangle$.

3. The meaning of the ansatz (7) is perhaps better clarified in the framework of the Fredholm integral equation. Suppose we have a Fredholm equation with symmetric positive kernel

$$|\psi\rangle = |g\rangle + \lambda \int \psi |\psi\rangle \quad (10)$$

the solution of which is
$$|\psi\rangle = \frac{R(\lambda)|g\rangle}{D(\lambda)}$$

where $D(\lambda)$ is a number, the Fredholm determinant. It is easy to see that the functional

$$\frac{\langle \psi | \psi \int \psi | \psi \rangle}{\langle \psi | \psi | \psi \rangle} \quad (11)$$

has maxima where it is equal to the inverse of the eigenvalues of λ (actually an absolute maximum corresponding to the smallest eigenvalue and then relative maxima which are absolute in the space of the functions orthogonal to the eigenfunctions corresponding to the eigenvalues of smaller size).

The eigenvalues are the zeros of $D(\lambda)$. If λ is an eigenvalue, then $R(\lambda)|g\rangle$ is an eigenfunction. $R(\lambda)|g\rangle$ looks like a linear combination of $(\psi)^n|g\rangle$, which is indeed the form of the ansatz (7). In the true solution when λ is equal to an eigenvalue $R(\lambda)|g\rangle$

depends on $|g\rangle$ through a normalization coefficient only, due to the factorization property of the solution. It is, however, apparent that the solution of the variational principle corresponding to (11) with the ansatz (7) and N finite will give an eigenvalue depending on $|g\rangle$. We can then ask for the best choice of $|g\rangle$ in a given subspace (the best one in the whole L_2 space corresponds of course to $|g\rangle$ equal to the eigenfunction). In terms of the Padé method language this procedure is equivalent to starting by considering a set of Fredholm equations obtained from Eq. (10) varying $|g\rangle$ in a given subspace, to construct for every equation the corresponding Padé approximant from the Neumann series, to find the poles by means of Eq. (5) and to choose as the best approximation the value of the pole which is stationary with respect to variations of $|g\rangle$. In general the best approximation will occur for a $|\bar{g}\rangle$ different from the inhomogeneous term of the integral equation in which one is actually interested.

As an example, let us specify the kernel $\mathcal{V}$ in a representation, for instance let the kernel be a continuous matrix $\mathcal{V}(x', x)$. We can choose as $|g\rangle$ a state having the representative $\delta(x-x_0)$. If the kernel is separable of rank 2, that is

$$\mathcal{V}(x', x) = \frac{\varphi_1(x')\varphi_1(x)}{\lambda_1} + \frac{\varphi_2(x')\varphi_2(x)}{\lambda_2}$$

the Padé approximant with $N=2$ is the exact solution ⁵⁾. One sees immediately, using Eq. (11), that even the Padé approximant with $N=1$ gives the exact eigenvalues when x_0 is such that $\varphi_1(x_0) = 0$ or $\varphi_2(x_0) = 0$, and that these values of x_0 make expression (11) stationary.

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4. Coming back to potential scattering, we conclude by suggesting to take the parameter k , which specifies the two-pion state in the ansatz (7) as a free parameter, different in general from $\sqrt{E}$. This extra free parameter can be used to improve the approximation by means of the variational principle corresponding to Eq. (8).

As a very simple example, let us consider a three-dimensional space well. We know that in the interior of the well the bound state wave function has the same form as the free wave function, namely $j_J(kr)$, but $k \neq \sqrt{E}$ (which would be imaginary), instead of $k = \sqrt{\lambda - |E|}$. If we put as an ansatz in Eq. (8) $|\psi\rangle = |\pi\pi kJ\rangle$, corresponding to the Padé approximant with $N=1$, the exact eigenvalues of λ will correspond to values of k for which Eq. (8) is stationary.

All we have said for potential scattering can be repeated for the Bethe-Salpeter equation, for instance in the ladder approximation, provided we replace in Eqs. (6), (7) and (8) $1/(H_0 - E - i\xi)$ by the two-particle propagators. If we take the B.S. equation in the form of an integral equation, we can argue as in Section 2. In this case the wave function in momentum space, corresponding to the inhomogeneous term of the integral equation, will depend on the two variables k and k_0 , the modulus of the space part and the fourth component of the relative momentum in the c.m. frame.

One can use the ansatz (7) in the variational principle (8) by allowing variations of k and k_0 . In this case, however, the independent variation of k and k_0 off the physical values $k = \sqrt{-m_\pi^2 + E^2/4}$, $k_0 = 0$, can also be thought of as the variation of the external masses m_1, m_2 off the physical values $m_1 = m_2 = m_\pi$ at fixed total energy, equal to E in the state $|\pi\pi J\sqrt{E}\rangle$ defining the ansatz (7) *).

*) Of course the ansatz (7) is poor at $E=0$ when it is convenient to choose in the ansatz a $O(4)$ symmetric state rather than an eigenstate of the angular momentum.

5. We argue that the prescription on the choice of the external masses should be also valid, in a variational sense, when one is searching for bound states in field theory by means of the Padé approximant constructed from the usual perturbative series. The matrix elements appearing in (6) are interpreted in the interaction representation, the states being dependent on time, i.e.,

$$\begin{aligned} \langle \psi^- | V | \psi^+ \rangle &\rightarrow \int dt \langle \psi^-(t) | V(t) | \psi^+(t) \rangle \\ \langle \psi^- | V \frac{1}{E + i\epsilon - H_0} V | \psi^+ \rangle &\rightarrow -i \int dt \int dt' \langle \psi^-(t) | V(t) \theta(t - t') V(t') | \psi^+(t') \rangle \\ &\text{etc.} \quad (12) \end{aligned}$$

(The matrix elements must be divided by the measure of the four volume.)

In order to obtain off-mass-shell as well as on-mass-shell matrix elements, we can consider a more general problem in which weak fields are also included. In our example each of the initial and final pions is replaced by a couple of leptons in a pseudoscalar state which are coupled to the strong source of the pion. At the end of the calculation we pick up the fourth order in the weak coupling constant. We will write for the states $|i\rangle$ and $|f\rangle$ appearing in (6): $|i\rangle = |\ell_1 \ell_2^J \sqrt{E}\rangle$, and $|f\rangle = |\ell_1' \ell_2'^J \sqrt{E}\rangle$.

The solution of the variational principle of Eq. (6) will express $\Psi^+(t)$ as the application of the operator $U^+(t)$ on the state $|i\rangle$

$$|\Psi^+(t)\rangle = U^+(t) |\ell_1 \ell_2^J \sqrt{E}\rangle \quad (13)$$

A formal expression for $U^+(t)$ is given by the perturbative expansion. The evaluation of Eq. (6) at the stationary point will reproduce the off-mass-shell scattering amplitude when the fourth order in weak interactions is picked up.

The homogeneous equation for a bound state, describing the time evolution in the interaction picture can be written as

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$$|\Psi(t)\rangle = -i \int_{-\infty}^t dt' V(t') |\Psi(t')\rangle \quad (14)$$

In order to specify a given energy level, we assign to $|\Psi(t)\rangle$ the form of the time dependence

$$|\Psi(t)\rangle = e^{i(H_0 - E)t} |\Psi(0)\rangle \quad (15)$$

where E is the bound energy. Then Eq. (14) becomes an eigenvalue equation. The variational principle, which is the relativistic form of Eq. (8), is obtained by stating that $|\Psi(t)\rangle$ makes stationary the expression :

$$\begin{aligned} (i)^2 \int dt \int dt' \langle \Psi(t) | V(t) \Theta(t-t') V(t') | \Psi(t') \rangle + \\ + i \int dt \langle \Psi(t) | V(t) | \Psi(t) \rangle \end{aligned} \quad (16)$$

where the dependence on time of $|\Psi(t)\rangle$ is an input of the problem and it is assigned as in Eq. (15). The Cini-Fubini ansatz, analogously to Eq. (7), corresponds to the trial form for $|\Psi(t)\rangle$

$$|\Psi(t)\rangle_{\text{trial}} = \sum_{n=1}^N a_n (-i)^{n-1} \int_{-\infty}^t dt' V(t') \int_{-\infty}^{t'} dt'' \dots \int_{-\infty}^{t^{(n-2)}} dt^{(n-1)} V(t^{(n-1)}) | \ell_1 \ell_2 \sqrt{E} \rangle \quad (17)$$

The energy E of the state $|\ell_1 \ell_2 \sqrt{E}\rangle$ is taken to be the bound state energy in order to satisfy Eq. (15).

From the variational principle, it follows an equation for $V(t)|\Psi(t)\rangle$, rather than for $|\Psi(t)\rangle$ directly. The ansatz (17) gives us a trial state of the form $V(t)O(t)|\ell_1 \ell_2 \sqrt{E}\rangle$, where $O(t)$ is the operator appearing in (17). The advantage of this ansatz is that when it is introduced in Eq. (16), it gives rise to an expression which can be calculated according to known rules, that is, one obtains a combination of Feynman diagrams.

A difficulty can arise when considering Eq. (16) with the ansatz (17), due to the appearance of disconnected diagrams. However, we expect that the bound states should appear as poles in the connected part of the off-mass-shell scattering amplitude. A device would be to consider Eq. (6) for $|i\rangle$ and $|f\rangle$ with slightly different values of the masses of the lepton couples. This defines the connected part of T . If the ansatz (17) for large N approaches the solution, Ψ^+ and Ψ^- being constructed starting from slightly different states, only connected diagrams must occur in the equations following from the variational principle, and in particular in the equations for the variation of (16), which express a pole of the general scattering amplitude. To support this reasoning, we note that the form (16) is stationary for independent variation of $\langle\Psi|$ and $|\Psi\rangle$, and they can be thought of as a priori different states, say $\langle\Psi_1|$ and $|\Psi_2\rangle$. In particular, if $V(t)|\Psi_1\rangle$ solves the homogeneous equation, the form (16) must be stationary for variation of $\langle\Psi_2|$ around values different from $|\Psi_1\rangle$. From this it follows that if the ansatz (17) approaches the wave function of a bound state, the connected part of (16) must have zero variation ^{*)}.

In conclusion, the variational principle can be used by varying independently the parameters e_i as well as the parameters which specify the state appearing in the ansatz. In the case, for instance, of the Bethe-Salpeter equation, the parameters are the masses of the external virtual particles for which the scattering amplitude, to be treated with the method of Padé approximants, is considered. We suggest to use the same dependence on the external masses when the Padé approximants are constructed from the perturbative series in field theory. In practice, the procedure is to construct the Padé approximants for a general off-mass-shell scattering amplitude, and to select as the best approximation to the eigenvalues of the coupling constant Λ (or of the bound energy if Λ is fixed) the zeros of Eq. (5), i.e., the poles of the Padé approximant, which are stationary for the variation of the external masses.

^{*)} The diagrams which contain bubbles on the external legs must, however, be taken into account, contributing to the appropriate order in the coupling constant Λ when the Padé approximants are constructed. They will be zero if the variational principle selects physical values for the external masses.

R E F E R E N C E S

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