A VARIATIONAL APPROACH TO OPERATOR AND MATRIX PADE APPROXIMATION. APPLICATIONS TO POTENTIAL SCATTERING AND FIELD THEORY

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A VARIATIONAL APPROACH TO OPERATOR AND MATRIX PADE APPROXIMATION. APPLICATIONS TO POTENTIAL SCATTERING AND FIELD THEORY

P. Kery

We define the operator and matrix Padé approxima
tion. We emphasise the fact that these approximants can be derived from the Schwinger variational principle. In potential theory, we shall show, using this variational aspect, that the matrix Padé approximation allow to reproduce the exact solution of the Lippman-Schwinger equation with a required accuracy taking only into account the knowledge of the first two coefficients in the Born expansion. The deep analytic structure of this variational matrix Padé approximation (hyper Padé approximation) is discussed.

1 Introduction

The convergence properties of the Padé approxima
tion in potential scattering have been studied for a long time [1]. It has been shown that if one takes into account a very high number of coefficients in the Born expansion an arbitrary accuracy can be reached.

Very important progress have been made after reali
ing that the Padé approximation could be derived from variational principles [2].

Using the Rayleigh-Ritz variational principle, Padé approximations have been derived which have allow
ed to increase deeply the accuracy of the calculation of bound states and resonances as well for the two body problem as for the three body problem or for the Bethe-Salpeter equation [3].

Another type of variational approximation has been defined by using the variational aspect of the operator and matrix Padé approximation [4]. It has
been shown that such a type of approximation allow to get incredibly accurate results in potential scattering [5], [6], [7].

We present here the variational Matrix Padé approximation method and proof its convergence in the case of non changing sign potentials. Numerical tests show that one get also convergence for any type of potential [5], [6], [7].

This Padé method (hyper Padé) is not a rational fraction approximation it allows for instance to reproduce deeper analytic structure such as algebraic cut.

As a consequence the variational matrix Padé approximation can be used in a competitive way with other standard methods for classical Schrödinger-like problems. Furthermore it can be extended to field theory and could allow to improve deeply the description of strong interaction particle physics using a minimal number of parameters [8].

2 The operator Padé approximation

2.1 Definition

Let $T(\alpha)$ be an operator analytic in $\alpha$ which can be expanded around $\alpha = 0$ in a formal power serie according to:

$$T(\alpha) = T_0 + \alpha T_1 + \alpha^2 T_2 + \ldots + \alpha^n T_n + \ldots$$

($2.1$) $T(\alpha)$ is a non commuting operators.

Due to this non commuting character one can a priori define several types of Padé approximants [9] such as: left, right or mixed Padé approximants

$$(2.2) \quad T(\alpha) = L_{Q_{n-1}}(\alpha) L_{P_{n}}(\alpha) = O(\alpha^{N+K+1})$$

$$(2.3) \quad T(\alpha) = R_{P_{n}}(\alpha) R_{Q_{n-1}}(\alpha) = O(\alpha^{N+K+1})$$
(2.4) $T(a) = \sum_{n=0}^{M} a^n = M(a) T(a) = 0(a^{N+1})$

One can prove that these three types of approximants are equal \([7], [9]\), and so we shall define the operator Pade approximant to $T(a)$ by:

(2.5) $[M/M] T(a) = \sum_{n=0}^{M} a^n = M(a) T(a) = 0(a^{N+1})$

The operator Pade approximants (O.P.A.) have the same covariance properties as the usual approximants. Furthermore one can prove that the O.P.A. to a direct sum of operators is the direct sum of the O.P.A. to each operator i.e.

(2.6) $T(a) = \sum_{i=1}^{N/M} T_i(a) = \sum_{i=1}^{N/M} T_i(a) = \sum_{i=1}^{N/M} T_i(a)$

2.2 The variational aspect of the operator Pade approximation

Consider the Lippman-Schwinger functional

\[ \mathcal{F}(V, V^*) = i \int_{t_0}^{t} dt' [V^*(t', t) H(t') + H(t') V(t', t_0)] \]

(2.7) $+ i \int_{t_0}^{t} dt' V(t', t) H(t') V(t', t_0)$

where $H(t)$ is the interaction hamiltonian and where $V$ and $V^*$ are arbitrary time dependent operators.

The Lippman-Schwinger variational principle \([10]\) states that:

(2.8) $\delta \mathcal{F}(V, V^*) = 0 \Rightarrow V = U(t, t_0)$

where $U(t, t_0)$ is the evolution operator between times $t$ and $t_0$. Letting $t_0 \rightarrow -\infty$ and $t \rightarrow +\infty$ one gets the $S$-scattering operator.
Using the Cini–Fubini ansatz [11], i.e. choosing for trial operator $V$ a linear combination (with operator coefficients) of the first $N$-terms of the Taylor expansion of $U(t,t_0)$ one can show that the formal solution of the Lippman–Schwinger variational principle is the $[N/N]$ O.P.A. to $U(t,t_0)$ [9]. Again if $t_0 \to +\infty$ and $t \to +\infty$ the $[N/N]$ O.P.A. to the S-scattering operator is solution of the Lippman–Schwinger variational principle.

### 2.3 The operator Padé approximation and the Lippman–Schwinger Equation

Let $K(E)$ be the scattering operator which is solution of the Lippman–Schwinger equation for an Hamiltonian $H = H_0 + \lambda V$

### (3.1) $K(E) = \alpha V + \alpha VG_0(E)K(E)$

with

### (3.2) $G_0(E) = \frac{1}{2}\left[(E+i\epsilon-H_0)^{-1} + (E-i\epsilon-H_0)^{-1}\right]$

The exact solution of this equation can be written in a formal way as:

### (3.3) $K(E) = \alpha V[1-\alpha VG_0(E)V]^{-1}V$

what is nothing but the $[1/1]$ O.P.A. to $K(E)$

### (3.4) $K(E) = [1/1]K(E)$

Such a result can be extended to semi-relativistic equations such as the Blankenbecler–Sugar equation [12] or to the Bethe–Salpeter equation in the ladder approximation.

### 3 The variational matrix Padé approximation

#### 3.1 Definition

All the results mentioned in the previous section are formal results as far as the operators $V$
are interested in act in an infinite dimensionnal Hilbert space. To compute an O.P.A. we need to invert an operator, this can be done only by discretizing the Hilbert space and so we can compute only a matrix Padé approximant.

Using the Lippman-Schwinger principle one can prove for potential scattering that the discretization points must be choosen in a variationnal way. We shall call such an approximation a variationnal matrix Padé approximation (V.M.P.A.).

The problem is now to look at the accuracy of this method and for that we shall study potential scattering. As it has already been mentionned if the number of discretization points was infinite we would get the exact solution to the Lippman-Schwinger equation, let us now look at what happen in the realistic case.

We shall call $q_i$ the discretization points of our Hilbert space ; $q_0$ is the center of mass momentum (on-shell point). We shall consider states $|q_i>$ with defined angular momentum and energy $\frac{q_i^2}{2m}$ ; we shall call $E_L$ the set of $|q_i>$ i.e. our discretized Hilbert space with $(L-1)$ off-shell points

\begin{equation}
E_L = \{|q_i>; i = 0, ..., L-1\}
\end{equation}

$E_L(E)$ will be the restriction of the scattering operator $K(E)$ to the discretized Hilbert space $E_L$.

### 3.2 The quasi-potential Theorem

Let $V$ be a positive and regular potential ($V(r) = 0(r^{-2+\epsilon})$ for $r \to 0$ and $V(r) = O(r^{-3-\epsilon})$ for $r \to \infty$ with $\epsilon > 0$). Let $E_{N,L}$ be the following space :

\begin{equation}
E_{N,L} = \{ (\sqrt{W}(\xi)V)^N \sqrt{V}|q_i>; m=0, ..., N-1; L=0, ..., L-1 \}
\end{equation}
and $P_{N,L}$ be the projector over the space $E_{N,L}$.

The $[N/N]$ matrix Padé approximant to $K_L$ is solution of a Lippman-Schwinger equation with a non local potential $V_{N,L} = \sqrt{V} V_{N,L} \sqrt{V}$.

The proof of this theorem can be found in reference [7]. This theorem has a deep physical meaning, indeed it allows to construct a quasi potential, i.e. a non local potential reproducing a given number of coefficients of the perturbative expansion.

3.3 The variational matrix Padé approximation in the case of non-changing sign potentials

If we increase $L$ we increase the number of vectors in the space $E_{N,L}$ i.e. for a given order of the approximation $[N/N]$ we just increase the number of off-shell points so that

$$E_{N,1} \subset E_{N,2} \subset \ldots \subset E_{N,L} \subset \mathcal{H}$$

where $\mathcal{H}$ is the infinite dimensional Hilbert space.

The above inequalities imply :

$$P_{N,1} < P_{N,2} < \ldots < P_{N,L} < \ldots < I$$

where we recall that $P_{N,L}$ projects over the space $E_{N,L}$.

$1$ is the identity over the Hilbert space.

As far as we are concerned with positive potentials ($V > 0$) we have

$$V_{N,1} < V_{N,2} < \ldots < V_{N,L} < \ldots < V$$

and due to the Feynman-Bellmann theorem, we get

$$\delta_{N,1} > \delta_{N,2} > \ldots > \delta_{N,L} > \ldots > \delta$$

where $\delta_{N,L}$ is the exact phase shift computed with the $V_{N,L}$ potential i.e.. taking into account the quasi-potential theorem.
The phase shift $\delta$ computed with the potential $V$ is given by

\[ \tan(\delta_{N,L}) = -q_0 <q_0|\frac{N/N}{K_L}|q_0> \]

The above relations show how to choose the off-shell momenta in a variational way indeed:

\[ \sup_{q_1,\ldots,q_{L-1}} \delta_{N,L} > \delta \]

Furthermore relation (3.10) show the convergence to the exact solution of the phase shifts computed through the V.M.P.A.

It was known for a long time that convergence can be obtained by increasing the order of the approximation i.e. through the knowledge of a larger number of coefficients of the perturbative expansion. Such a convergence can also be obtained at a given order of the approximation by increasing the size of the matrix i.e. the dimension of the discretized Hilbert space. This is a far easier task from a practical point of view. The numerical examples given below will illustrate the fact that convergence can be obtained using only a very small number of off-shell points.

Let us notice that:

i) the same kind of results can be obtained for $V < 0$ with opposite inequalities;

ii) an identical proof can also be given in the case of singular potentials using the regulator as a variational parameter [13].

In the case of sign changing potentials one must notice that they cannot be described through the ordinary $[1/1]$ Padé approximation indeed, in this case, a change of sign can only occur in the denominator which
means that the phase shift goes to 90° and not to 0°. We have no rigorous proof of convergence of the V.M.P.A. in the case of such potentials however numerical examples show also a convergence to the exact solution and a conjecture has been emitted [5] to characterize the choice of off-shell momenta by taking the values of the $q_i$ corresponding to the extremum the closest to the on-shell value $q_0$.

3.5 Numerical examples

The practical way to compute variationnal matrix Padé approximants can be found in references [5], [6], [7]. The V.M.P.A. method has first been applied to study square wells potential. In the case of a single well it has been proved [14] that with one off-shell point the variationnal choice of the momentum correspond to the momentum inside the well and reproduce numerically the exact result. With two square wells [5] one has studied the variationnal choice of the off-shell point in the case of a sign changing potential, the results illustrate the conjecture presented above.

We show here a table which summarize our result [7] in the case of a continuous exponential potential $V = V_0 e^{-\mu r}$, this table illustrate the convergence of our method.

We have used the same notations as in reference [15] in which the convergence had been studied by increasing the order of the approximation. Here we always compute a [1/1] Padé approximant including one or two off-shell momenta. In the case of a weakly attractive or repulsive potential only one off-shell momentum allows to get very accurate results. Using two off-shell points, we can even describe very strongly attractive potentials, for example with two bound
states at threshold. The method has also been applied to study double exponential sign changing potentials and the results confirm our conjecture for the choice of the discretization points [7].

4 The analytic structure of the variational matrix Padé approximation

The matrix Padé approximation is a rational fraction approximation but this is no longer true for the variational matrix Padé approximation (hyper Padé approximation).

Indeed, let us consider for example the computation of a phase shift through a \([1/1]\) matrix Padé approximation to the K-matrix with 1 off-shell point i.e.

\[
\delta(a, q_0, q) = \arctan[- q_0 <q_0|\hat{\rho}|\hat{q}_0>]
\]

\(\delta(a, q_0, q)\) is a rational fraction in the coupling constant \(a\).

When we consider the V.M.P.A. we eliminate the off-shell momentum \(q\) through:

\[
\delta(q, a, q_0) = 0 \quad \Rightarrow \quad q = q(a, q_0)
\]

Then \(\delta(q, a, q_0)\) is a function with a deeper analytic structure that a rational fraction.

As an example consider a square wall

\[
V = aV_0 \quad \text{if} \quad r < r_0
\]

\[
= 0 \quad \text{if} \quad r > r_0
\]

It has been proved [14] that the \([1/1]\) V.M.P.A. allows to reproduce exactly the \(1S_0\) phase shift i.e. the function:

\[
\frac{\gamma a \sin(q_0^2 + aV_0r) \cos(q_0r) - \sqrt{q_0^2 + aV_0r} \cos(q_0^2 + aV_0r) \sin(q_0r)}{q_0 \sin(q_0^2 + aV_0r) \sin(q_0r) + \sqrt{q_0^2 + aV_0r} \cos(q_0^2 + aV_0r) \cos(q_0r)}
\]
5 Conclusion

As we have seen the variational matrix Padé approximation is a very confident method to study any Schrödinger-like problem. Using the variational aspect of the approximation, we have shown that for potential scattering the method allows to reproduce the exact results with any required numerical accuracy computing only the first two coefficients of the perturbative expansion.

In field theory this method could be applied in the same way and could allow to describe strong interaction physics such as for example nucleon-nucleon scattering.

For this kind of problem the Green's function in the center of mass system can be parametrized through

\[
\sqrt{\frac{E}{2} + \omega, p} \quad \sqrt{\frac{E}{2} - \omega', p'}
\]

\[
\sqrt{\frac{E}{2} - \omega, -p} \quad \sqrt{\frac{E}{2} - \omega', -p'}
\]

If we neglect spin the partial wave expansion of this Green's function read

\[
G(s, \omega, \omega', p, p', \cos \theta) = \sum J G^J(s, \omega, \omega', p, p') P_J(\cos \theta)
\]

where \( \theta \) is the scattering angle in the center of mass system. The partial wave coefficient can be computed by

\[
G^J(s, \omega, \omega', p, p') = \langle \omega, p | G^J(J) | \omega', p' \rangle
\]

The perturbative expansion of \( G^J(s) \) is given by Feynman's diagrams

\[
G^J(s) = a G(1)^J(s) + a^2 G(2)^J(s) + \ldots
\]
The $[1/1]$ Padé approximant to $CJ(s)$ is then:

$$[1/1] CJ(s) = \infty^{(1)} J(s) [C^{(1)} J(s) - \infty^{(2)} J(s)]^{-1} C^{(1)} J(s)$$

Although we cannot prove any rigorous result we can hope that a variational choice of the discretization points can also be done here in field theory. In this case we could have for the first time a good description of the strong interaction physics with a minimal number of parameters.

Table

1So phase shift for an exponential potential $V(r) = -V_{ee}^{-\mu^2}$ (phase shifts are given in degrees)

<table>
<thead>
<tr>
<th>$\nu$</th>
<th>Ordinary Padé</th>
<th>Variational 2x2 Matrix Padé</th>
<th>Exact solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>- 6.10</td>
<td>-9.237</td>
<td>-9.242</td>
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<tr>
<td>0.5</td>
<td>-54.952</td>
<td>-43.734</td>
<td>-43.771</td>
</tr>
<tr>
<td>1.0</td>
<td>-56.975</td>
<td>-76.726</td>
<td>-76.861</td>
</tr>
<tr>
<td>2.0</td>
<td>-71.029</td>
<td>-110.862</td>
<td>-111.801</td>
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### Case $g = -1$

<table>
<thead>
<tr>
<th>$-iv$</th>
<th>Ordinary Padé</th>
<th>Variational 2x2 Matrix Padé</th>
<th>Variational 3x3 Matrix Padé</th>
<th>Exact solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>.1</td>
<td>-3.506</td>
<td>-3.572</td>
<td>-3.574</td>
<td>-3.574</td>
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<tr>
<td>1.</td>
<td>-22.620</td>
<td>-23.281</td>
<td>-23.308</td>
<td>-23.308</td>
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### Case $g = +1$

<table>
<thead>
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<th>Ordinary Padé</th>
<th>Variational 2x2 Matrix Padé</th>
<th>Variational 3x3 Matrix Padé</th>
<th>Exact solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>.5</td>
<td>35.882</td>
<td>38.088</td>
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<td>38.278</td>
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<td>1.</td>
<td>32.005</td>
<td>32.525</td>
<td>33.618</td>
<td>33.633</td>
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<td>2.</td>
<td>22.051</td>
<td>22.809</td>
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### Case $g = +8$

<table>
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<th>Variational 2x2 Matrix Padé</th>
<th>Variational 3x3 Matrix Padé</th>
<th>Exact solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>.1</td>
<td>168.600</td>
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<td>292.257</td>
<td>302.143</td>
</tr>
<tr>
<td>.5</td>
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<td>1.</td>
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<td>183.027</td>
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<td>2.</td>
<td>74.290</td>
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### Case $g = +10$

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<th>Ordinary Padé</th>
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<th>Variational 3x3 Matrix Padé</th>
<th>Exact solution</th>
</tr>
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<tr>
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<td>226.235</td>
<td>231.011</td>
</tr>
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<td>2.</td>
<td>77.660</td>
<td>161.248</td>
<td>171.353</td>
<td>174.073</td>
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</table>
References


   Turchetti G. (same reference).


6 Benofy L., Gammel J., contribution to this conference.
