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UNAMBIGUOUS RESULTS FROM VARIATIONAL MATRIX PADE APPROXIMANTS.

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Maciej PINDOR *

Centre de physique Théorique,
C.N.R.S. Marseille

ABSTRACT : Variational Matrix Padé Approximants are studied as a non-linear variational problem. It is shown that although a stationary value of the Schwinger functional is a stationary value of VMPA, the latter has also another stationary value. It is therefore proposed that instead of looking for a stationary point of VMPA, one minimizes some non-negative functional and then one calculates VMPA at the point where the former has the absolute minimum. This approach, which we call the Method of the Variational Gradient (MVG) gives unambiguous results and is also shown to minimize a distance between the approximate and the exact stationary values of the Schwinger functional.

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Permanent Address : Institute of Theoretical Physics, Warsaw University, ul. Hoza 69, 00-681 WARSAVA (Poland).

Postal Address : Institute of Theoretical Physics, Warsaw University, ul. Hoza 69, 00-681 WARSAVA (Poland).

1. Introduction

Variational Matrix Padé Approximants [1] can be regarded as a bridge between the two apparently distinct approaches to computational problems of quantum physics -the perturbative and the variational ones.

Therefore it seems justified to expect, and simple examples from the potential quantum mechanics [2] and quantum field models [3,4] support such expectation, that the method could evolve into an efficient and convenient computational tool of quantum physics.

Although the method can give exact results in some simple cases [5], it does not, in general provide a unique answer [2,8] and therefore it needs a detailed analysis to see what are possible sources of ambiguities and, eventually, to eliminate them.

In Section 2 we outline the method of VMPA and point out that it is equivalent to some non-linear variational problem.

In Section 3 we analyze the non-linear functional related to the scattering and find equations that must be satisfied if the functional has to be stationary. We show then which of those equations corresponds to the stationary point of the original functional (the Schwinger functional).

In Section 4 we point out that when a conditional variational problem is considered, an approach different from looking for a conditional stationary point should give better results and we formulate the new approach in a form of a search for absolute minimum of a new non-negative functional.

2. VARIATIONAL MATRIX PADE APPROXIMANTS

We are interested in solving an integral equation for some integral operator $K(z)$, the formal shape of the equation being

$$K(z) = gV + gVG_0(z)K(z) \tag{1}$$

In the potential scattering gV is a potential, $K(z)$ can either be K or T matrix, and then $G_0(z)$ is the free Green function either for standing or for outgoing free waves, correspondingly.

In the relativistic scattering, the Bethe-Salpeter equation has the same form with the necessary re-interpretation of symbols.

The formal solution of (1) is :

$$K(z) = \frac{1}{1-gVG_0(z)}\, gV = gV\frac{1}{V-gVG_0(z)V}V \tag{2}$$

It is well known (e.g. [6]) that a matrix element of between any two state vectors, can be found from the Schwinger variational principle which states that a unique stationary value of the functional :

$$R_{\alpha\beta}(\psi,\psi') = \langle\alpha|V|\psi\rangle + \langle\psi'|V|\beta\rangle - \langle\psi'|V-gVG_0V|\psi\rangle \tag{3}$$

is just $\frac{1}{g}\langle\alpha|K(z)|\beta\rangle$; (We do not show explicitly a dependence of $R_{\alpha\beta}$ on z).

If we take, in the case of the potential scattering

$|\alpha\rangle = |p_\alpha, l\rangle$, $|\beta\rangle = |p_\beta, l\rangle$ -free spherical standing waves of definite energy, matrix elements of K become the off-shell values of the K-matrix (if $G_0 = G_0^P$ -principal value Green function) for definite angular momentum:

$$\langle p_\alpha, l | K(z) | p_\beta, l\rangle = K_l(p_\alpha, p_\beta; z)$$

and for $p_\alpha = p_\beta = \sqrt{2mz}$ $(z>0)$ we have :

$$K_l(p, p; \frac{p^2}{2m}) = -\frac{1}{2mp} \tan\delta_l(\frac{p^2}{2m})$$

Padé Approximants appear when we look for a constrained stationary value of $R_{\alpha\beta}$, namely if we restrict ψ, ψ' to a subspace $H_{L,N}$ of the full space of state vectors H , $H_{L,N}$ being spanned by

$$\{\varphi_i\}_0^{L-1}, \{(G_0V)\varphi_i\}_0^{L-1}, \ldots\ldots \{(G_0V)^{N-1}\varphi_i\}_0^{L-1} \;;\; \alpha, \beta \in \{\varphi_i\}_0^{L-1} \qquad (4)$$

(We shall not consider here the transformation performed by introducing $V^{\frac{1}{2}}$ (see e.g. [1]) - it is straightforward only if the potential does not change sign, otherwise the operator considered is nonselfadjoint and also matrix elements of K cannot be expressed as matrix elements of the resolvent of that operator ; As a result the formulae are not simpler than they were without this transformation).

One can show then that [7]:

$$\underset{\psi,\psi' \in H_{L,N}}{\text{stationary value}}\; R_{\alpha\beta}(\psi,\psi') = \langle\alpha\,|[N-1/N]_{\frac{1}{g}K^L}(g)|\beta\rangle = R^{L,N}_{\alpha,\beta} \qquad (5)$$

where K^L is $P_L K(g;z) P_L$ - a restriction of K to a subspace spanned by $\{\varphi_i\}_0^{L-1}$ (P_L projects onto this subspace).

It is however obvious that we must also have :

$$R^{L,N}_{\alpha,\beta} = \langle\alpha|[0/1]_{\frac{1}{g}K^{L,N}}(g)|\beta\rangle = \langle\alpha|VP_{L,N}\frac{1}{P_{L,N}(V-gVG_0V)P_{L,N}}P_{L,N}V|\beta\rangle \quad (6)$$

where $P_{L,N}$ projects onto $H_{L,N}$ and $K^{L,N}$ is a restriction of K to this subspace (the formula (6) follows directly from (5) when we take all vectors of the form (4) for φ_j 's, and when we calculate $[0/1]$ by hand).

The method of VMPA exploits now the fact that for any finite L and N , $R^{L,N}_{\alpha\beta}$ depends on all φ_j 's (and not only on α and β). One can therefore change φ_j $(\neq \alpha,\beta)$ and look for a stationary value of $R^{L,N}_{\alpha\beta}$. It can be shown [1] that $R_{\alpha\beta}$ is a stationary value of $R^{L,N}_{\alpha\beta}$, however without a detailed analysis of the latter (what is the content of the next section) nothing can be told whether it has other stationary values. In fact the numerical analysis of this nonlinear functional has shown, for sign changing potentials [2,8], that there were other stationary values. Although one of them was very close to $R_{\alpha\beta}$ it was not clear how should this value be selected.

3. ANALYSIS OF THE NONLINEAR FUNCTIONAL

In the following we shall consider, for simplicity only :

$$R_{oo}^{L,1} = \langle\varphi_o|VP_L\frac{1}{P_L(V-gVG_oV)P_L}P_LV|\varphi_o\rangle = R_{oo}^L(\varphi_i) \tag{7}$$

and we shall comment on more general cases in the conclusions. For the moment we shall assume that the set $\{\varphi_i\}_o^{L-1}$ is orthonormal -however later we shall present the formulae for a more general case. If φ_i's are orthonormal, then

$$R_{oo}^L(\varphi_i) = \sum_{kl}\langle\varphi_o|V|\varphi_k\rangle W_{kl}^{-1}\langle\varphi_l|V|\varphi_o\rangle \tag{8}$$

and

$$W_{ij} = \langle\varphi_i|V-gVG_oV|\varphi_j\rangle \tag{9}$$

(if φ_i's are not orthonormal, a matrix of the inverse operator is not the inverse matrix of the operator itself - see Appendix A for the corresponding formulae).

To study stationary points of R_{oo}^L we consider

$$|\varphi_k\rangle = |\varphi_n^o\rangle + \varepsilon\delta_{kn}|\psi\rangle \tag{10}$$

and expand R_{oo}^L around $\varepsilon = 0$ keeping only first two terms :

$$R_{oo}^L(\varepsilon) \cong R_{oo}^L + \varepsilon R'(\psi) \tag{11}$$

It is easy to find that

$$R'(\psi) = \sum_l\langle\varphi_o|V|\varphi_l\rangle W_{ln}^{-1}\cdot\langle\psi|(V|\varphi_o\rangle - W\sum_{rk}|\varphi_r\rangle W_{rk}^{-1}\langle\varphi_k|V|\varphi_o\rangle +$$

$$+\sum_l W_{nl}^{-1}\langle\varphi_l|V|\varphi_o\rangle\cdot(\langle\varphi_o|V - \sum_{rk}\langle\varphi_o|V|\varphi_k\rangle W^{-1}\langle\varphi_r|W)|\psi\rangle \tag{12}$$

Let us now observe that if the change of φ_i's given by (10) preserves their orthonormality, then $|\psi\rangle$ must be orthogonal to all $|\varphi_i^*\rangle$ - and in fact vectors entering scalar products with in (12) are automatically orthogonal to H_L.

The condition for stationarity of R^L_{oo} is

$$R'(\psi) \underset{\psi}{\equiv} 0$$

and it can happen only if either:

$$V|\varphi_0\rangle - (V - gVG_0V)P_L \frac{1}{P_L(V-gVG_0V)P_L} P_L V|\varphi_0\rangle = 0 \tag{13}$$

or :

$$\langle\varphi_n| \frac{1}{P_L(V-gVG_0V)P_L} P_L V|\varphi_0\rangle = 0 \tag{14}$$

Now, we can easily see what (13) means :

$$\frac{1}{V-gVG_0V} V|\varphi_0\rangle = P_L \frac{1}{P_L(V-gVG_0V)P_L} P_L V|\varphi_0\rangle \tag{15}$$

and

$$\langle\varphi_0|V \frac{1}{V-gVG_0V} V|\varphi_0\rangle = \langle\varphi_0|VP_L \frac{1}{P_L(V-gVG_0V)P_L} P_L V|\varphi_0\rangle = R^L_{oo} \tag{16}$$

Therefore (13) is just the condition for the stationary value of R^L_{oo} to be the stationary value of R_{oo} , i.e. $\frac{1}{g}\langle\varphi_0|K(z)|\varphi_0\rangle$

However (14) means something different and is equivalent to

$$\frac{1}{P_L(V-gVG_0V)P_L} P_L V|\varphi_0\rangle = \alpha|\varphi_0\rangle \tag{17}$$

To see that this condition can easily be satisfied even if (16) does not hold let us observe that it can also be expressed in the form :

$$(V - gVG_0V)|\varphi_0\rangle = \frac{1}{\alpha} V|\varphi_0\rangle + |\eta\rangle$$

where $P_1|\eta\rangle = 0$.

If $V|\varphi_0\rangle$ is not, accidentely, an eigenvector of $1 - gVG_0$, and $V|\varphi_0\rangle$ and $|\varphi_0\rangle$ are not parallel we can write

$$(V - gVG_0V)|\varphi_0\rangle = \beta V|\varphi_0\rangle + |\chi\rangle \tag{18}$$

where $\langle\varphi_0|\chi\rangle = 0$. Then of course :

$$\beta = \frac{\langle\varphi_0|V - gVG_0V|\varphi_0\rangle}{\langle\varphi_0|V|\varphi_0\rangle} \tag{19}$$

If we now choose all other φ_i's orthogonal to $|\chi\rangle$, we have, in agreement to (17) :

$$\beta = \frac{1}{\alpha} = \frac{\langle\varphi_0|V|\varphi_0\rangle}{R^L_{00}}$$

However, from (18) we have :

$$R^L_{00} = \langle\varphi_0|V\frac{1}{V - gVG_0V}V|\varphi_0\rangle + \frac{R^L_{00}}{\langle\varphi_0|V|\varphi_0\rangle}\langle\varphi_0|V\frac{1}{V - gVG_0V}|\chi\rangle$$

and in order to have $R^L_{00} = \frac{1}{g}\langle\varphi_0|K(z)|\varphi_0\rangle$ we need :

$$\langle\varphi_0|V\frac{1}{V - gVG_0V}|\chi\rangle = 0 \tag{20}$$

and this condition does not depend on φ_i's $i \neq 0$.

For a given $|\chi\rangle$ depending, as it can be seen from its definition (18), only on V , VG_0V and $|\varphi_0\rangle$, there are infinitely many vectors orthogonal to it, and so (17) can easily be satisfied even if (20) is not.

We conclude that in general, R^L_{oo} will have two stationary values :

$$\langle\varphi_o| V \frac{1}{V - gVG_oV} V |\varphi_o\rangle \qquad \text{and} \qquad \frac{\langle\varphi_o|V|\varphi_o\rangle^2}{\langle\varphi_o| V - gVG_oV |\varphi_o\rangle}$$

and as it is shown in the Appendix non-orthonormality of vectors φ_i does not change anything.

In the practical application of VMPA we are unable, of course, to vary φ_i's over the whole space H but we rather change them over some multiparameter manifold :

$$|\varphi_n\rangle = |\varphi_n(\lambda)\rangle$$

Then, however, $|\psi\rangle$ is not arbitrary :

$$|\varphi_n(\lambda)\rangle = |\varphi_n(\lambda_o)\rangle + (\lambda - \lambda_o)|\varphi'_n(\lambda_o)\rangle$$

(for simplicity we consider the dependence of φ's on one parameter only, but the generalization is obvious).

Now the condition for stationarity of R^L_{oo} on the manifold is

$$R'(\varphi'(\lambda_o)) = 0 \tag{21}$$

and it does not need a great imagination to guess that if R^L_{oo} has two stationary values in the full space of its arguments (and at least one of the values is achieved on infinitely many different points) it will have many, if the arguments are somehow constrained. We could somehow improve the situation demanding that :

$$\langle\varphi'(\lambda)|V|\varphi_0\rangle - \langle\varphi'(\lambda)|(V-gVG_0V)P_L \frac{1}{P_L(V-gVG_0V)P_L} P_L V|\varphi_0\rangle = 0 \qquad (22)$$

what is sufficient but not a necessary condition (21) to hold, and which is satisfied at the true stationary point, and generally not at the second one.

Unfortunately (22) is also not the very good condition. It depends e.g. on $|\varphi'(\lambda)\rangle$, i.e. on a "shape" of the manifold over which we vary φ_i's. It may happen, therefore, that although our manifold approaches very closely a point at which (13) is satisfied, still (22) is satisfied only at a point of the manifold lying far away. Moreover it may happen that (22) has, still, more than one solution and it is impossible to guess which one gives R^L_{00} closest to $\frac{1}{g}\langle\varphi_0|K(z)|\varphi_0\rangle$.

4. THE NEW VARIATIONAL CONDITION

The objections raised at the end of the last section can be resolved if we observe that if (13) is the condition that our approximation to $\frac{4}{g}\langle\varphi_0|K(z)|\varphi_0\rangle - R^L_\omega$ - will be exact, and it will not, generally, be the case on the manifold over which we vary φ_i's, we can probably pick up the point on the manifold closest to the solution of (13) if we minimize the modulus of :

$$|\gamma(\varphi_i)\rangle = V|\varphi_0\rangle - (V-gVG_0V)P_L\frac{1}{P_L(V-gVG_0V)P_L}P_LV|\varphi_0\rangle \tag{23}$$

The subtle point lies in the fact that modulus of $|\gamma(\varphi_i)\rangle$ may not exist if V is more singular than r^{-1} at the origin. We may, however, observe that the condition (13) is equivalent to

$$|V|^{-1/2}|\gamma(\varphi_i)\rangle = 0 \tag{24}$$

and look for a minimum of :

$$\mathcal{G}(\varphi_i) = \langle\gamma(\varphi_i)|\frac{1}{|V|}|\gamma(\varphi_i)\rangle \tag{25}$$

The full expression for $\mathcal{G}$ is

$$\mathcal{G}(\varphi_i) = \langle\varphi_0|M|\varphi_0\rangle - \langle\varphi_0|(|V|-g|V|G_0V)P_L\frac{1}{P_L(V-gVG_0V)P_L}P_LV|\varphi_0\rangle +$$

$$-\langle\varphi_0|VP_L\frac{1}{P_L(V-gVG_0V)P_L}P_L(|V|-gVG_0|V|)|\varphi_0\rangle +$$

$$+\langle\varphi_0|VP_L\frac{1}{P_L(V-gVG_0V)P_L}P_L(|V|-g|V|G_0V-gVG_0|V| + \tag{26}$$

$$+g^2VG_0|V|G_0V)P_L\frac{1}{P_L(V-gVG_0V)P_L}P_LV|\varphi_0\rangle$$

For potentials which are sufficiently regular at the origin we could have taken directly $\langle\gamma(\varphi_i)|\gamma(\varphi_i)\rangle$ but the form (26) emerges naturally if we use correctly the transformation with $\sqrt{|V|}$ described e.g. in [1].

Our proposal is, therefore, that instead of looking for a point on the manifold at which R^L_{oo} is stationary, we should look for a point minimizing $\mathcal{G}(\varphi_i)$ there. $\mathcal{G}$ is non negative and it is relatively easy to find numerically its absolute minimum.

One could argue, however, that this approach neither does not necessarily select a point on the manifold at which R^L_{oo} is closest to $\frac{1}{g}\langle\varphi_o|K(z)|\varphi_o\rangle$ — $\mathcal{G}$ could have many minima and if our manifold does not approach the solution of (13) very closely, we can again have absolute minimum of $\mathcal{G}$ on the manifold to lie far from the "best" point (although at least in that favorable situation we shall not miss it).

To see to what extent are these objections serious, let us calculate $|R^L_{oo} - \frac{1}{g}\langle\varphi_o|K(z)|\varphi_o\rangle|^2$:

$$|\langle\varphi_o|VP_L \frac{1}{P_L(V-gVG_oV)P_L} P_LV|\varphi_o\rangle - \langle\varphi_o|V\frac{1}{V-gVG_oV}V|\varphi_o\rangle|^2 =$$

$$= |\langle\varphi_o|[VP_L \frac{1}{P_L(V-gVG_oV)P_L} P_LV - V\frac{1}{V-gVG_oV}V]|\varphi_o\rangle|^2 =$$

$$= |\langle\varphi_o|V\frac{1}{V-gVG_oV}[(V-gVG_oV)P_L \frac{1}{P_L(V-gVG_oV)P_L} P_LV - V]|\varphi_o\rangle|^2 =$$

$$= |\langle\varphi_o|V\frac{1}{V-gVG_oV}|\gamma(\varphi_i)\rangle|^2 \leq \langle\varphi_o||V||\varphi_o\rangle \cdot$$

$$\cdot \langle\gamma(\varphi_i)|\frac{1}{V-gVG_oV}|V|\frac{1}{V-gVG_oV}|\gamma(\varphi_i)\rangle$$

and finally

$$|R^L_{oo} - \frac{1}{g}\langle\varphi_o|K(z)|\varphi_o\rangle|^2 \leqslant \mathcal{G}(\varphi_i)\cdot\langle\varphi_o|V|\varphi_o\rangle \left\| |V|^{\frac{1}{2}} \frac{1}{V-gVG_oV} |V| \frac{1}{V-gVG_oV} |V|^{\frac{1}{2}} \right\| \qquad (27)$$

Although we are, unfortunately, unable to calculate the norm of the operator in (27), neither we can find an upper bound to it from a knowledge of matrix elements of V and VG_oV on H_L, we see that finding φ_i's minimizing $\mathcal{G}(\varphi_i)$ gives us the "safest" value of R^L_{oo} on the manifold.

5. CONCLUSIONS

Summarizing we propose that the method of VMPA should be modified in the following way : after finding

$$\langle \varphi_0 | [\widetilde{1/1}]_{\frac{1}{g}K^L}(g) | \varphi_0 \rangle = \langle \varphi_0 | V P_L \frac{1}{P_L (V - g V G_0 V) P_L} P_L V | \varphi_0 \rangle = R^L_{00}$$

one should not look for stationary value of it with respect to φ_i's, but one should find the absolute minimum of $\mathcal{G}(\varphi_i)$ (given by (26)) and calculate R^L_{00} on φ_i's realizing this minimum.

One can easily repeat our considerations for $R^L_{\alpha\beta}$, $\alpha \neq \beta$ and we shall not do it here.

Also higher orders of perturbation can be included in this scheme : introducing $v = \mathrm{sgn}\, V$ we can express $\mathcal{G}$ by matrix elements of

$$\langle \varphi_i | V P_{L,N} \frac{1}{P_{L,N} (V - g V G_0 V) P_{L,N}} P_{L,N} V | \varphi_k \rangle - \langle \varphi_i | [N-1/N]_{\frac{1}{g}K^L}(g) | \varphi_k \rangle$$

Considering instead of $H_{L,N}$, $H_{L,N}$ spanned by vectors of the form (4) influences only a shape of our manifold. In this way, also modification of vectors φ_i in agreement to the proposal given in [5] does not present any basic difficulties.

Analoguous considerations can be performed for bound states (or rather for values of g giving bound states at a given energy). Although in that case, no spurious stationary points analoguous to the one defined by (14) seem to appear it also seems reasonable to look rather for a minimum of a "variational gradient" like $|\gamma(\varphi)\rangle$, which can also in this case be calculated, than to consider the constrained stationary problem for g's defined by (2.38) in [1]. However, in that case we were unable to find, up to now, a formula analoguous to (30).

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APPENDIX A

If φ_i are not orthogonal we must use the full formula :

$$R^{L}_{oo} = \langle\varphi_0|VP_L \frac{1}{P_L(V-gVG_0V)P_L} P_L V|\varphi_0\rangle = \langle\varphi_0|VP_L \frac{1}{P_L W P_L} P_L V|\varphi_0\rangle \qquad (A.1)$$

Now we define P' through

$$P_L(\varepsilon) \cong P_L(0) + \varepsilon P' = P_L + \varepsilon P' \qquad (A.2)$$

and then

$$R'(\psi) = \langle\varphi_0|VP' \frac{1}{P_L W P_L} P_L V|\varphi_0\rangle - \langle\varphi_0|VP_L \frac{1}{P_L W P_L}(P'WP_L +$$

$$+ P_L W P')\frac{1}{P_L W P_L} P_L V|\varphi_0\rangle + \langle\varphi_0|VP_L \frac{1}{P_L W P_L} P' V|\varphi_0\rangle \qquad (A.3)$$

but as :

$$P_L = \sum_{ij} |\varphi_i\rangle F^{-1}_{ij} \langle\varphi_j| \qquad (A.4)$$

$(F^{-1}_{ji} = [F_{mn}]^{-1}_{ji}$ and $F_{mn} = \langle\varphi_m|\varphi_n\rangle$,

it is easy to find that :

$$P'(\psi) = \sum_{i} \left[(1-P_L)|\psi\rangle F^{-1}_{ni} \langle\varphi_i| + |\varphi_i\rangle F^{-1}_{in} \langle\psi|(1-P_L)\right] \qquad (A.5)$$

and finally :

$$R'(\psi) = \sum_i \langle\varphi_0|VP_L \frac{1}{P_L W P_L}|\varphi_i\rangle F^{-1}_{in} \langle\psi|(1-P_L)(V|\varphi_0\rangle - WP_L \frac{1}{P_L W P_L} P_L V|\varphi_0\rangle) +$$

$$+ \sum_i F^{-1}_{in} \langle\varphi_i| \frac{1}{P_L W P_L} P_L V|\varphi_0\rangle (\langle\varphi_0|V - \langle\varphi_0|VP_L \frac{1}{P_L W P_L} P_L W) \cdot \qquad (A.6)$$

$$\cdot (1-P_L)|\psi\rangle$$

The factor $(1-P_L)$ is in fact unnecessary because the content of the round bracket is automatically orthogonal to H_L . The condition (14) takes now the form :

$$\sum_i F_{ni}^{-1} \langle \varphi_i | \frac{1}{P_L (V - gVG_0V) P_L} P_L V | \varphi_0 \rangle = 0 \qquad \text{(A.6)}$$

but it is immediately seen to be also equivalent to (17).