SCHWINGER'S VARIATIONAL PRINCIPLE IN SCATTERING THEORY*

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We give a detailed account on the application of the Schwinger variational principle (SchVP) for the evaluation of operator Padé approximates (OPA's). OPA's can be considered in their simplest "one-loop" (ladder) form as solutions of scattering equations but allow for a more natural transition to quantum field theory beyond ladder approximation. Therefore methods for their evaluation are of high interest. One of these methods is the SchVP which we study in the special case of elastic nucleon-nucleon scattering in terms of the Blankenbecler-Sugar equation. Since exact proofs of convergence for the SchVP cannot be found in general, the intention of our paper is to give by a detailed study of this complex example a justification for the application of the SchVP in even more complex situations. Applying the SchVP, it is shown that relatively simple and quite precise approximations for the T-matrix elements can be constructed valid for the whole energy range under consideration.

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1. Introduction

The Schwinger variational principle (SchVP) [1] is described in textbooks of quantum mechanics (see e.g. [2]) and in particular also its application to the calculation of phase shifts [2, 3] in potential scattering.

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Nevertheless its merits seem not to be appreciated properly if in [2], under "Extensions to Complex Collisions", p. 863, we read as final conclusion "In any case its applications are rather limited". The purpose of the present paper is to demonstrate the opposite.

The suggestion of our method to evaluate the SchVP has been made earlier [4], resulting in a "variational operator Padé approximation". In contrary to the "standard" procedure of constructing a functional of stationarity for the partial wave amplitudes directly, which depends on trial functions in configuration space, in our procedure we start with the Green functions in momentum space and use the "off-shell" momenta as variational parameters. Moreover the functional which we construct, is not directly related to the phase shifts. Its absolute minimum determines the off-shell momenta at which to evaluate the (discretized) "matrix Padé approximate".

Proofs of convergence for the variational methods are in general difficult to find. In potential theory proofs of convergence have e.g. been given in [5] for the SchVP, but only for potentials with definite sign. In more complex situations like nucleon-nucleon (NN) scattering, taking into account all spin complications, general proofs seem out of reach and therefore it is highly desirable to have at least available for such a complicated case a detailed numerical study of a "realistic" partial wave analysis. This is the purpose of the present work: to explore in a more calculable example the application of our procedure, i.e. the model should not be as trivial as square wells or potentials of definite sign, it should be more accessible than the elaborate Bethe-Salpeter equation (BSE) but it should also reproduce the phase shifts properly, what we call "realistic". In the case of the BSE [4] in particular, we were unable, because of the amount of CPU time involved, to find the solution for the 3S_1 phase shift by means of the SchVP, which should be the first problem to be solved if one wants to demonstrate the quality of a new method. In particular in this coupled channel problem it is far from trivial, what the one variational quantity should be, yielding simultaneously two phase shifts and one mixing parameter. How this can be achieved, will be demonstrated.

In order to be able to perform a complete analysis of the NN phase shifts and to answer such as the mentioned questions, we give in this paper a detailed study of the phase shifts in terms of the simpler Blankenbecler—Sugar (BbS) equation, the known solutions of which we reproduce by the application of the SchVP. Even if such analysis cannot substitute proofs of convergence, we think that it adds some more justification for the applicability of the SchVP in scattering processes.

The explicit numerical evaluation of the principle, in the form we proposed it, uses much computer time and it cannot therefore be its purpose to substitute standard methods for the numerical evaluation of the Lippmann—

-Schwinger equation (or relativistic generalizations) like matrix inversion or the application of ordinary Padé approximations [6]. Rather the idea behind our approach is to investigate in detail in how far the method is applicable to the summation of any strong coupling theory. Indeed it is our conjecture, that in contrary to one of the possible approaches to scattering problems in relativistic quantum field theories (QFT) like the Bethe-Salpeter equation (BSE), it is much more natural to formulate the QFT in terms of "operator Padé approximations", for the explicit evaluation of which we use the SchVP.

Our paper is organized as follows. In Section 2 we describe our general procedure based on the SchVP. In Section 3 we discuss the application to the BbS equation and give some technical details of the NN scattering. Section 4 contains our results and in Section 5 we summarize our philosophy.

2. A general formulation of scattering theory in Quantum Field Theory

As starting point we consider the (amputated) Green functions for a relativistic scattering theory in momentum space. The (renormalized) onshell values of these yield the S-matrix elements. In a two-particle elastic scattering problem (to which we confine here for simplicity) the S-matrix is symmetric under exchange of ingoing and outgoing particles, *i.e.* under exchange of the corresponding momenta. In this sense we consider the Green functions as symmetric operators in some Hilbert space \mathcal{H} (labelled by off-shell momenta), which posses a formal power series expansion (loop-expansion) of the form

$$T = T_0 + T_1 + T_2 + \cdots (1)$$

Since in the following applications we consider the T-matrix, we call our operators T as well.

The usual formulation of the scattering problem in QFT is the following: take the on-shell values of series (1) term by term and sum it — which does not work in strong coupling theories. Even using "ordinary" Padé approximants, one would need to calculate in general higher than one-loop orders — which is almost out of reach. Here we propose a different approach: consider the contributions $T_i(i=1,2,3,\cdots)$ in the above expansion indeed as operators and sum the operator series by using "operator Padé approximants" (OPA's), which in lowest order yields

$$T_{\text{OPA}}^{(1)} = T_0 \left[T_0 - T_1 \right]^{-1} T_0 \tag{2}$$

and which can be continued in a natural manner to higher orders, e.g.

$$T_{\text{OPA}}^{(2)} = T_0 + T_1 [T_1 - T_2]^{-1} T_1,$$
 (3)

taking into account the next ("two-loop") order. The on-shell matrix elements are then to be taken only after the "summation" of the operator series, *i.e.* we want to obtain on-shell matrix elements from the r.h.s. of (2) and (3), respectively, as will be explained below.

Before entering the technicalities of this approach, let us first demonstrate that already on the level of the lowest order of the OPA (see (2)) with T_0 = Bornterm and T_1 = direct box diagram, the proposed approach is formally equivalent to the BSE in ladder approximation — and correspondingly of course its reductions like the BbS or nonrelativistically the Lippmann-Schwinger equation.

Inserting the direct box diagram $T_1 = T_0 S T_0 \equiv D$ with S the two-nucleon propagator into (2) and expanding $[T_0 - T_1]^{-1}$ in powers of T_0 , one obtains:

$$T_{\text{OPA}}^{(1)} = T_0 + T_0 S T_0 + T_0 S T_0 S T_0 + \cdots, \tag{4}$$

which is the ladder series, taking the on-shell matrix elements after the expansion.

Already at this stage we want to point out that, provided the above approach is manageable, it appears more natural than the BSE when going to a full theory. The kernel of the BSE is defined as the sum of the two particle (nucleon) irreducible diagrams. Adding diagrams in a strongly interacting QFT, it makes more sense to add those of the same order than adding e.g. the crossed box diagram as a "correction" to the Bornterm. This is what we advertise: adding all one-loop diagrams in T_1 , one only adds contributions of the same order. Assuming — as we want to demonstrate in the present paper — that the evaluation of (2) works for $T_1 = D$, one can hope that it also works when taking for T_1 the full one-loop contribution. In this manner also the inclusion of contributions considered particularly important in certain problems, like the crossed box diagram in NN scattering [6], is possible in a very natural way. Thus we exploit as much as possible the one-loop approach, which is nowadays feasible [7], i.e. before entering the tremendous work of two-loop calculations, we here propose to go off-shell in the described manner.

To clarify our point of view even more, we want to stress that the OPA's are constructed in such a manner that their expansion reproduces the first terms in the loop-expansion properly (i.e. $T_{\mathrm{OPA}}^{(1)} = T_0 + T_1 + \cdots, T_{\mathrm{OPA}}^{(2)} = T_0 + T_1 + T_2 + \cdots$, etc.), while the further terms need not have any meaning, i.e. in general they will not even be higher order Feynman diagrams. In view of this, the fact that the lowest order OPA, $T_{\mathrm{OPA}}^{(1)}$, produces the ladder series (4), i.e. it solves the BSE in ladder approximation, is a very welcome result, as trivial as the formal algebra to obtain it may be. Thus we consider the lowest order $T_{\mathrm{OPA}}^{(1)}$ already as a very effective starting point for the

summation of the perturbation theory. The Padé philosophy behind our procedure does not keep us from including e.g. the two-loop ladder diagram in T_2 in the next order even if it is contained in the formal expansion of $T_{\mathrm{OPA}}^{(1)}$ already. This is so because of the above reasons we give no particular meaning to any finite expansion of the OPA's beyond the one used for its construction. The relevant objects of our approach are only the OPA's and clearly in the infinite order limit they do reproduce the perturbation expansion, at least formally.

The Schwinger variational method enters the evaluation of the desired on-shell matrix elements in the following manner [1]: starting from the functional

$$R_{\alpha\beta}(\psi,\psi') = \langle \psi'|T_0|\beta\rangle + \langle \alpha|T_0|\psi\rangle - \langle \psi'|T_0 - T_1|\psi\rangle , \qquad (5)$$

(considering only $T_{\text{OPA}}^{(1)}$, Equ. . (2), in what follows) we perform independent variations with respect to the states $|\psi\rangle$ and $|\psi'\rangle$. A simple formal algebra then shows that the stationary value of (5) is the sought matrix element

$$T_{\text{OPA}}^{\alpha\beta} = \langle \alpha | T_{\text{OPA}} | \beta \rangle , \qquad (6)$$

where $|\alpha\rangle$ and $|\beta\rangle$ are considered as on-shell states.

The practical realization of the above principle is performed in two steps:

1) In the first step one confines oneself to a finite-dimensional subspace $\mathcal{H}_L \subset \mathcal{H}$ of the Hilbert space in which the T-operator acts, *i.e.*

$$\mathcal{H}_L = P_L \mathcal{H}, \quad P_L^2 = P_L, \tag{7}$$

with P_L a projection operator. Assuming that \mathcal{H}_L is spanned by some vectors $|\phi_1\rangle = |\alpha\rangle, |\phi_2\rangle = |\beta\rangle, |\phi_3\rangle, \cdots, |\phi_L\rangle$, it has been shown [8] that the stationary value of $R_{\alpha\beta}$ obtained with $|\psi\rangle$, $|\psi'\rangle \in \mathcal{H}_L$ only is given by the "discretized" operator Padé approximate, *i.e.* a "matrix Padé" (MP):

stat value
$$R_{\alpha\beta}(\psi, \psi') = \left\langle \alpha \left| T_0 P_L \frac{1}{P_L (T_0 - T_1) P_L} P_L T_0 \right| \beta \right\rangle$$

$$= R_{\alpha\beta}^L (\phi_3, \dots, \phi_L). \tag{8}$$

2) In the second step one has to find an optimal way of how to determine the states $|\phi_3\rangle, \dots, |\phi_L\rangle$, which in our case are characterized by certain

off-shell momenta of the momentum space Green functions under consideration. As has been proven in [4], the condition for stationarity of $R_{\alpha\beta}$ is the vanishing of the vector

$$\langle \gamma_{\alpha} | = \langle \alpha | T_0 \left[I - P_L \frac{1}{P_L(T_0 - T_1)P_L} P_L(T_0 - T_1) \right]. \tag{9}$$

and similarly $\langle \gamma_{\beta} |$, *i.e.* the stationary point of $R_{\alpha\beta}^{L}$ is achieved when $\langle \gamma_{\alpha} | = 0$ or $\langle \gamma_{\beta} | = 0$. Under this condition $R_{\alpha\beta}^{L}$ also coincides with the stationary point of the Schwinger functional, *i.e.*

$$R_{\alpha\beta}^{L} = T_{\text{OPA}}^{\alpha\beta} \,, \tag{10}$$

which to obtain was our goal.

An "intuitive" way to understand the above is the following: consider the difference of the on-shell matrix elements of the OPA and the matrix Padé, *i.e.*

$$\Delta \equiv \left| \left\langle \alpha \left| T_0 \frac{1}{T_0 - T_1} T_0 \right| \beta \right\rangle - \left\langle \alpha \left| T_0 P_L \frac{1}{P_L (T_0 - T_1) P_L} P_L T_0 \right| \beta \right\rangle \right|
= \left| \left\langle \alpha \left| T_0 \frac{1}{T_0 - T_1} \left[I - (T_0 - T_1) P_L \frac{1}{P_L (T_0 - T_1) P_L} P_L \right] T_0 \right| \beta \right\rangle \right|
= \left| \left\langle \phi_{\alpha} | \gamma_{\beta} \right\rangle \right|,$$
(11)

with

$$\langle \phi_{\alpha} | = \langle \alpha | T_0 \frac{1}{T_0 - T_1}. \tag{12}$$

From

$$|\langle \phi_{\alpha} | \gamma_{\beta} \rangle| \le ||\phi_{\alpha}|| \cdot ||\gamma_{\beta}||, \tag{13}$$

we immediately conclude that $\langle \gamma_{\alpha} | = 0$ or $\langle \gamma_{\beta} | = 0$ provides the solution of the problem to calculate the on-shell matrix element of T_{OPA} .

In general, however, it will not be possible to achieve $\langle \gamma_{\alpha} | \equiv 0$. The best we can achieve is to minimize the norm $\|\gamma_{\alpha}\|$ of $\langle \gamma_{\alpha} |$. Even if we have no information about $\|\phi_{\alpha}\|$ (see (12)), from (11) and (13) we conclude that in this case we have obtained the best possible approximation to our problem. Thus the procedure in practice will be to begin with a low number (1 or 2) of "trial states" and look for the minimum of $\|\gamma_{\alpha}\|$ as a function of their position. Increasing the number of trial states should yield a lower minimum of $\|\gamma_{\alpha}\|$ but finally should leave the value of the investigated matrix element stable. Observe that

$$P_L |\gamma_{\alpha}\rangle = 0, \qquad (14)$$

i.e. the more trial states are introduced, the more zeroes "contribute" in the calculation of the norm of $\langle \gamma_{\alpha} |$ (see also (20) below) and this is at lest a qualitative explanation of how $\|\gamma_{\alpha}\|$ can be made smaller and smaller by introducing more and more trial states. The real problem in this procedure is to find the minimum of $\|\gamma_{\alpha}\|$ for a given number of trial states. This is so in particular if a large number of trial states is necessary, since in general the calculation of $\|\gamma_{\alpha}\|$ will involve a relatively large amount of CPU time already for one set of trial states as will be seen in the next Section.

3. Application to the Blankenbecler-Sugar equation for NN scattering

The Blankenbecler-Sugar equation in the form used here is reduced from the BSE

$$\Phi(p, p_0, \alpha) = G(p, p_0, \alpha; \hat{p}, 0, \kappa) \\
-\frac{i}{2\pi^2} \int dq dq_0 \sum_{\beta\gamma} G(p, p_0, \alpha; q, q_0, \beta) S(q, q_0, \beta, \gamma) \Phi(q, q_0, \gamma), (15)$$

where κ stands for the partial wave under consideration, G is the kernel and S the two-nucleon propagator. For the detailed meaning of the summation indices see [6, 9]. The elements of S are expressed in terms of S_{++}, S_{--}, S_{ee} and S_{eo} , the indices here referring to positive and negative energies (and "even" and "odd", respectively), for details see [6, 10]. In the BbS reduction the positive energy two-nucleon propagator is represented as a dispersion integral in the total energy squared such that in our case we have $S_{++} \sim \delta(q_0)$ [11]. The q_0 -integration in (15) can then be performed and only q_0 -even contributions remain. For the two-nucleon propagator this means $S_{eo} = 0$ and we can write

$$S_{--} = \left(\frac{E - E(q)}{E + E(q)}\right)^{2} S_{++}$$

$$S_{ee} = \frac{E - E(q)}{E + E(q)} S_{++}. \tag{16}$$

Thus also of the kernel G only those elements even in q_0 are kept. The kernel remains otherwise the same as in [6], *i.e.* it is a superposition of the relevant boson exchanges. The equation under consideration in this approximation finally reads:

$$\Phi(p,0,\alpha) = G(p,0,\alpha;\hat{p},0,\kappa)
+ \frac{1}{\pi} \int_0^\infty dq \sum_{\beta,\gamma} G(p,0,\alpha;q,0,\beta) S(q,0,\beta,\gamma) \Phi(q,0,\gamma), (17)$$

with

$$S(q,0,1,1) = S_{++} = \frac{1}{2} \frac{1}{E(q) - E - i\epsilon},$$
 (18)

and summation is only over q_0 -even states. The number of on-shell states is given by s=1 for J=0 and $L=J\neq 0$ and s=2 for the coupled triplet states.

The obtained equation with the chosen couplings [11] etc. reproduces the NN phase shifts properly for elastic scattering. The details of this reproduction are not so relevant here; for us it is only important that the chosen potential is "realistic" and we have a reasonable basis to test our approximation procedure.

First we have to construct the MP with $T_0 = G$ and $T_1 = GSG$, the direct box diagram, i.e. we calculate these with discretized external off-shell momenta to obtain the corresponding matrices. For each pair of off-shell points, however, due to the spin complications and those from the inclusion of the positive and negative energy states, we have to take into account already a whole "spin-matrix" as building block, the dimension of which depends on the partial wave under consideration: for J = 0 (J the total angular momentum) their dimension is $d_s = 3$, for $L = J \neq 0$ (L the orbital angular momentum) $d_s = 4$ and for coupled triplet states with $J \neq 0$ $d_s = 6$. Thus we construct matrices of the size $(s + d_s \cdot (L-1)) \times (s + d_s \cdot (L-1))$, with L-1 the number of off-shell points, from which we have to calculate the matrix Padé, the physical elements of which (i.e. the upper left $s \times s$ matrix) yields the physical phase shift at the given energy. The reason not to take matrices of size $(d_s \cdot L) \times (d_s \cdot L)$ for the calculation of the MP's, is that also in the BSE or the BbS equation, there are no on-shell states with negative energies involved.

In the next step we have to calculate for the given set of off-shell momenta our variational quantity

$$\|\gamma_{\alpha}\|^2 = \int dq \sum \gamma^2(q; p_1 = \hat{p}, p_2, \dots, p_L),$$
 (19)

with

$$\gamma^{2}(q = p_{i}; p_{1} = \hat{p}, p_{2}, \dots, p_{L}) = 0 \quad (i = 2, \dots L),$$
 (20)

according to (14).

In (19) summation is over "spin" indices and integration over the off-shell momentum q like in (17). Here \hat{p} is the modulus of the on-shell momentum and α characterizes the partial wave. (19) clearly shows why our procedure is so CPU time consuming: to evaluate $\|\gamma_{\alpha}\|^2$ one has to calculate (9) for each integration point in the above integral. This then yields $\|\gamma_{\alpha}\|^2$ only for a specific set of off-shell points and one must search for the

minimum of $\|\gamma_{\alpha}\|^2$ as a function of these in order to determine the off-shell momenta with which finally to calculate the MP to obtain the phase shift.

It should be mentioned that too few integration points for the numerical integration of (19) can produce spurious absolute minima and lead to wrong values of the phase shifts. Therefore we had to make sure that the number of integration points was large enough to stabilize the positions of the absolute minima. In general 24 Gaussian points were sufficient.

There is one peculiarity concerning the coupled triplet states: since two physical states couple, except for J=0 where we have only the 3P_0 -wave, we obtain from the 2×2 on-shell matrix two phaseshifts: ${}^3(J-1)_J$, ${}^3(J+1)_J$ and one mixing parameter ϵ_J . It is not unique in this case, what to take as "variational quantity". Writing (see (11) and [4])

$$\Delta = \left| \left\langle \gamma_{\alpha} \left| \frac{1}{T_0 - T_1} \right| \gamma_{\beta} \right\rangle \right| , \qquad (21)$$

we do not only have one vector squared, but we have to "minimize" the 2×2 matrix

$$\begin{pmatrix}
\left\langle \gamma_{1} \left| \frac{1}{T_{0} - T_{1}} \right| \gamma_{1} \right\rangle & \left\langle \gamma_{1} \left| \frac{1}{T_{0} - T_{1}} \right| \gamma_{2} \right\rangle \\
\left\langle \gamma_{2} \left| \frac{1}{T_{0} - T_{1}} \right| \gamma_{1} \right\rangle & \left\langle \gamma_{2} \left| \frac{1}{T_{0} - T_{1}} \right| \gamma_{2} \right\rangle
\end{pmatrix} \equiv \begin{pmatrix}
g_{11} & g_{12} \\
g_{21} & g_{22}
\end{pmatrix}$$
(22)

and we have to define what we mean by that. One option, e.g., would be to minimize separately g_{11} to calculate $\delta_{3(J-1)_J}$, g_{22} to calculate $\delta_{3(J+1)_J}$ and $|g_{12}|$ to calculate ϵ_J . But this does not necessarily correspond to the coupling of the two channels. Therefore we propose to take only one variational quantity, namely the norm of the matrix (22), i.e.

$$N \equiv g_{11}^2 + 2g_{12}g_{12}^* + g_{22}^2, \qquad (23)$$

which yields according to $||g_{12}||^2 \le ||g_{11}|| \cdot ||g_{22}||$

$$N \leq \left\| \frac{1}{T_0 - T_1} \right\| (\gamma_{11} + \gamma_{22})^2, \tag{24}$$

with $\gamma_{ii} = \langle \gamma_i | \gamma_i \rangle$ (i=1,2). Thus we will take $\gamma_{11} + \gamma_{22}$ as variational quantity to obtain simultaneously all three physical parameters in the coupled channel system.

4. Results

Before entering the details of our results, we shortly describe the way of searching for the minimum of our variational quantities. The first observation is that looking at the minimum of the norm of $\langle \gamma_{\alpha}|$, what we need to calculate are the Born (T_0) and Box (T_1) contributions in a twofold manner (see (9)): firstly we need matrix elements $\langle p|T_i|q\rangle(i=0,1)$ with both momenta p and q taking discretized values, which are indeed our variational parameters (specified formally by the projection operator P_L) and secondly we need the matrix elements with the momentum p discretized and q being the integration variable in (19), for which we take Gaussian integration with 24 mesh points in general.

The crucial observation now is that these matrix elements are the building blocks to calculate $||<\gamma_{\alpha}||$, independently of how many off-shell points as variational parameters are in fact used: thus, dumping such sets $\langle p_l | T_i | q \rangle$ $(p_l \in p_1, p_2, \cdots p_L)$ and q Gaussian), one can use it in the construction of $||<\gamma_{\alpha}||$'s for any arbitrary number of variational parameters. Moreover, to guarantee repetition of p_l 's and in this way saving for this computation as much execution time as possible, we always performed the search on a fixed grid of p_l 's, taking for them multiples of stepsize m/64 in general (m the nucleon mass), i.e. $p_l = \frac{l}{64}m$, $(l = 1, 2, \cdots)$. Only close to a minimum the stepsize was decreased occasionally to improve the result.

To accelerate finding of a minimum we furthermore applied the simplex method [12], adapted to the situation that we search on a k-dimensional grid (k = L - 1) instead of a continuous space. We recall that the simplex search algorithm starts from a simplex formed from k+1 vertices (in a kdimensional space) and searches for a minimum basically by reflecting the vertex corresponding to the maximum value of the function under consideration with respect to the hyperplane spanned by the remaining k points. If at the new point a lower value of the function is found, the former vertex is rejected and a new simplex is formed by the old k points and the new one. If, however, the new value is lower than the lowest one of the original simplex, another point is taken at a distance from the hyperplane of reflection twice as large as the former one. If the value at the reflected point is higher than the highest one, the simplex is shrinked with ratio 1:2 around the vertex corresponding to the smallest value of the function. In this way the simplex moves in space towards the minimum, shrinking in a narrow valley leading down and expanding if descent is fast. When our simplex reached the size of our grid's stepsize, such that it could not be shrinked anymore, we performed a refined search in this area, decreasing the stepsize down to m/256. To make sure that we found the global minimum, after finding a local minimum, we restarted the search with a simplex having one vertex in the minimum found and other vertices generated randomly. The process was interrupted, when the new search found the same minimum several (usually two or three) times.

Finally we present our results in Figs 1-5 and Tables I-III. γ^2 as given

in the following, is always meant as the "normalized" one, i.e. γ^2/γ_0^2 , where γ_0^2 is obtained from the Bornterm only. In detail our results are:

- 1) In Figs 1-3 we show for various partial waves γ^2 as well as the phaseshift at $E_{\text{Lab}} = 100 \text{ MeV}$ as a function of one off-shell momentum p as variational parameter (in units of m/64). The minimum of γ^2 is indicated by a vertical line and so is the phaseshift, calculated from the MP with the corresponding off-shell momentum. The dotted horizontal line is the "exact" value of the phaseshift, obtained by the application of ordinary Padé approximates to the BbS equation. Compared to the strong variation of the phaseshift in the considered range of the one off-shell momentum, the variational principle picks in general a fair approximation. It is interesting to note, that the value obtained in this manner is practically never a stationary value of the phaseshift itself, though one of the stationary values is mostly somewhat better. As has been demonstrated, however, in [4], where a very strong square well potential was investigated, this can only be considered as an accident. Amazingly we can observe already here — as will also be confirmed later — that it is the ${}^{1}S_{0}$ partial wave, which is the easiest to obtain by our procedure, i.e. the phaseshift is relatively smooth as a function of the off-shell momentum and the minimum of γ^2 is quite deep (see Fig. 2).
- 2) Since obviously the approximation with one off-shell momentum is not good enough, we present in Tables I-III the corresponding results with higher numbers of off-shell momenta as variational parameters. As a general remark we can state that, as expected, the ${}^{\bar{3}}S_1$ -coupled channel system (see Table I) is the most difficult one. To obtain a precision of the phaseshifts with an error < 10 in the whole energy range, we had to perform a search with 5 off-shell momenta (L = 6). This was in particular necessary for the low energies (< 50 MeV, closest to the bound state), while for the energies ≥ 100 MeV, four off-shell momenta gave already results of the same accuracy. This latter case also demonstrates very nicely the final stability of our procedure: increasing the number of off-shell momenta from four to five, γ^2 drops (though not drastically), but the phaseshifts obtained in both cases differ only by less than 0.20 for these larger energies. For the lower energies we expect the same kind of stability if we would perform searches with even more off-shell momenta, which we avoided, however, due to the increasing CPU time involved. For the purpose, we have in mind here, namely to demonstrate that the proposed method works for "realistic" problems, we consider our results in every respect convincing.

This is confirmed even more if we now look at the higher partial waves. With four off-shell momenta (L=5), the largest error for the 1S_0 is $\approx 0.3^0$

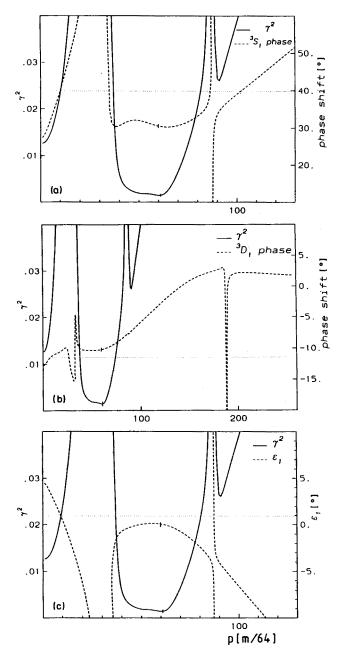


Fig. 1. For the 3S_1 -coupled channel system γ^2 and the phaseshifts are shown for $E_{\rm Lab}=100$ MeV as function of one off-shell momentum p [m/64] as variational parameter. The minima of γ^2 are indicated by vertical lines and also the phaseshifts calculated from the "matrix Padé" at the corresponding off-shell momentum; the horizontal vertical line represents the "exact" value. (a) 3S_1 , (b) 3D_1 , (c) 4S_1 .

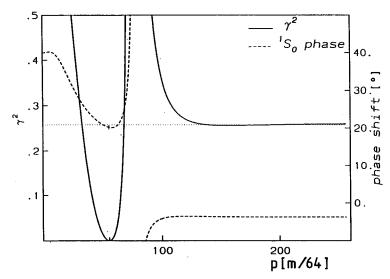


Fig. 2. Same as Fig. 1 for the ${}^{1}S_{0}$ phase shift.

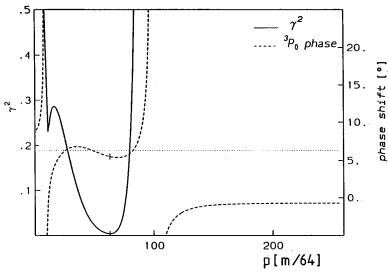


Fig. 3. Same as Fig. 1 for the 3P_0 phase shift.

(see Table II) and the stability of the phaseshift with increasing number of off-shell momenta as well as the decrease of γ^2 even at the lower energies is much better than that for the 3S_1 coupled channel system. Similarly for the 3P_0 (Table III): the error for L=5 is even less than 0.1^0 , only γ^2 is not so low as for the 1S_0 (remember that we give the normalized γ^2), but the stability of the phaseshift is really excellent.

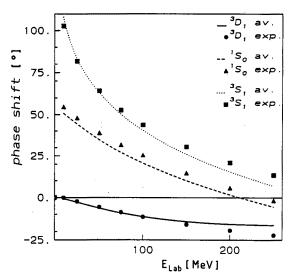


Fig. 4. The 3S_1 , 3D_1 and 1S_0 phaseshifts calculated from "averaged" MP's with four and five off-shell momenta as variational parameters, respectively (see the corresponding tables), in comparison with experimental data taken from [13].

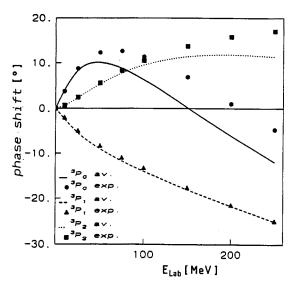


Fig. 5. Same as Fig. 4 for the 3P_0 , 3P_1 and 3P_2 phaseshifts. The "averaged" off-shell momenta ([m/64]) are for the 3P_1 : 33,68,125,200 and for the 3P_2 : 24,56,97,149. The largest deviations from $\delta_{\rm BBS}$ are 0.30 (for the larger energies) and 0.050, respectively.

For the higher partial waves we present our results less detailed. For the 3P_1 they were as well of the same convincing quality and the ones for the 3P_2 - coupled channel system show that our choice of $\gamma_{11} + \gamma_{22}$ as variational quantity (see (24)) appears to be the right one to obtain all three coupled phaseshifts with one variational quantity as in the case of the 3S_1 -coupled channel system (see Fig. 5 for some further details concerning these two phase shifts). Finally we find the surprising result for the 1P_1 that we obtain a good phaseshift but γ^2 is really dropping only very slowly, for which we don't understand the reason — in particular since the 1S_0 , which is of similar type, gives easily a relatively small γ^2 , as already discussed above.

Finally Tables I-III also show that the off-shell momenta, obtained in the process of the search for the minimum of γ^2 are surprisingly almost independent of the energy (see also [4]) and mainly depend on the partial wave under consideration, which allows us to construct for each partial wave a relatively simple approximation by choosing some set of "averaged" off-shell momenta (see Tables I-III) for the whole energy range. The results of this approximation are presented in Figs 4 and 5, where the phaseshifts calculated from the "averaged" MP are shown in comparison with experimental data, taken from [13]. The deviations of the averaged results from the ones obtained with specific searches are only relevant for the S-waves (see Tables I and II) at low energies. Moreover, the slow and systematic change of the off-shell momenta with the energy could be taken into account in a search, which would in fact drastically accelerate our procedure. Tables I and II for the S-waves (${}^3S_1: L=6$ and ${}^1S_0: L=5$) indicate that finally all off-shell momenta slightly increase with energy. Thus, changing the energy stepwise and taking such property into account, the changes of all off-shell momenta would be in one direction only (all increasing or all decreasing, respectively) and change only in relatively small steps. In this way the method would become even for the S-waves pretty fast. Figs 4 and 5 also demonstrate the fact that we are indeed dealing with a "realistic" problem.

5. Summary

We have shown that it is possible to solve the BbS equation by summing the ladder series with the help of an OPA even in the case of the 3S_1 phase shift, evaluating it by means of the SchVP — and indeed it turned out that the 3S_1 is a much harder problem than that of the higher partial waves. While for the 3S_1 , in particular at the lower energies, at least five off-shell momenta as variational parameters are needed, only one or two give already almost sufficient results for the higher partial waves.

The intention behind our procedure is not to substitute standard methods to solve integral equations but rather to develop a general approach

to sum the perturbation theory of a strongly coupled QFT. If the Padé approach is to be successful, it is first of all necessary to show in practice by evaluating explicit examples that it nevertheless solves known scattering equations. Since even for these proofs of convergence for the SchVP cannot be found in complex cases, the only remaining possibility is to test in as much detail as possible the procedure in numerical examples. The BbS approach appears as a case where a complete analysis of the partial wave scattering equations could be performed with a still reasonable computational effort. Therefore, because of missing proofs in general, we performed this numerical analysis, which finally was quite successful. We hope that our method will be applied with similar success in the evaluation of more complex models of QFT (for first attempts see [14]). Indeed, as has been explained, it appears to be the most natural way to include other higher order loop contributions than just direct boxes and higher rung ladders. If the proposed method can be considered as a manageable procedure to solve scattering equations, however, one can hope that it will also yield correct answers in more complete approaches to QFT. Even if our method is quite involved in certain cases, the surprising energy-independence of the off-shell momenta (variational parameters) obtained in the process of the search for a minimum of γ^2 allows in any case to construct quite precise approximations for the T-matrix elements valid over the whole energy range under consideration by simply performing the search for one energy, 100 MeV e.g., and use the corresponding off-shell momenta for all other energies. Moreover, as has been discussed, the slow and systematic change of the off-shell momenta can be used in a search to make the method fast even for the S-waves. In this sense we believe that the SchVP can be of great use in further calculations and may well compete with the direct, brute force matrix inversion.

What concerns models for the application of our procedure, e.g. a gauge field model with ρ - and ω -mesons as gauge fields, extending the linear σ -model, has been proposed [15], which should contain the essential ingredients of low energy hadron interactions. Even if QCD is considered as the "final" theory of strong interactions, the proper approach to low energy physics is still an unsolved problem. Taking into account the physical particles with finally as little phenomenological ad hoc assumptions (like "formfactors", e.g.) as possible should be a worthwhile approach.

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TABLE I

the BBS-equation [11] with the phase δ_m obtained at the off-shell point(s) $p_i[m/64]$, where $\|\gamma\|^2 \equiv \gamma^2$ takes its minimum value $\gamma^{L=2,3,...,6}$. L is the number of momenta (L-1) off-shell). Coupled triplet ${}^3S_1 + {}^3D_1$ phaseshifts: comparison for various energies E_{Lab} of the phaseshift δ_{BBS} obtained from

$E_{Lab}[MeV]$		10	25	50	75	100	150	200	250
		104.19	80.98	61.52	49.11	39.80	25.89	15.43	7.02
	3D_1	684		-6.35	-9.22	-11.45	-14.40	-	-16.37
	61	910	1.27	1.22	1.06		0.79	0.78	0.85
L=2	p_1	118	64	62	62	09	50	20	20
	$\gamma^{L=2}$	$2.62 \ 10^{-3}$	$7.39\ 10^{-4}$	$7.93\ 10^{-4}$	$7.39\ 10^{-4}\ 7.93\ 10^{-4}\ 1.04\ 10^{-3}$	-	$2.32 10^{-3}$	$1.44\ 10^{-3}\ 2.32\ 10^{-3}\ 2.76\ 10^{-3}\ 3.10\ 10^{-3}$	$3.10\ 10^{-3}$
	δ _m ³ S ₁		61.00	47.30	37.72			11.57	5.72
				·		ı	1	-16.51	-23.34
	1.3	0.306	2.48					-2.91	-3.18
L=3	p_1, p_2	56,83	56,84	55,84	54,69	29,57	34, 59	41,61	42,64
	$\gamma^{L=3}$	$5.13 10^{-4}$	2.5	$2.18 10^{-4}$	2.9	$2.10\ 10^{-4}$	$2.02 10^{-4}$	2.1	4.81 10-4
	δ_m 3S_1	76.36	61.65	47.71	38.25	31.49	19.12	11.17	4.33
			-2.72	-5.94		-11.44	-14.70	ı	-19.98
	61			1.47	0.54	92	-1.80	-2.50	-2.77
L=4	p1, p2, p3	7, 49, 110	6, 49, 117	5, 50, 115	33, 59, 92	7, 49, 110 6, 49, 117 5, 50, 115 33, 59, 92 32, 59, 126 2, 49, 102 7, 49, 100 11, 49, 96	2, 49, 102	7, 49, 100	11, 49, 96
	$\gamma^{L=4}$		2.10 10-4 1.39 10-4	$1.06\ 10^{-4}$	1.06 10-4 9.17 10-5	8.20 10-5	$1.32 10^{-4}$	$1.18\ 10^{-4}$	$1.22\ 10^{-4}$
	δ _m ³ S ₁	105.74	80.55	59.74		29.92	23.86	14.22	5.77
	" "D1		-2.80	-6.00	•	-11.29	-14.03	-15.66	-16.15
	£1			0.69			0.10	0.69	1.16

TABLE I (continued)

[
18,40 63,128 3.91 10-5 6.71 -16.73 0.57	16,44,68 158,187 2.13 10-5 6.79 -16.44 0.69	11, 37, 57 103, 144 4.19 10 ⁻⁵ 6.85 -16.25 0.78
16,40 63,127 3.42 10 ⁻⁵ 15.31 -16.04 0.51	15, 43, 68 157, 185 1.92 10 ⁻⁵ 15.36 -15.91 0.53	11, 37, 57 103, 144 3.33 10 ⁻⁵ 15.34 -15.72 0.63
15,40 62,127 2.94 10 ⁻⁵ 25.99 -14.51	12, 40, 65 120, 146 1.80 10—5 26.12 —14.23	1, 37, 57 103, 144 72 10 ⁻⁵ 25.98 -14.23
12,41 61,122 2.74 10 ⁻⁵ 40.60 -11.35	11, 38, 56 89, 127 89, 127 1.77 10 ⁻⁵ 40.44 -11.31 0.59	57 11, 37, 57 11, 37, 57 11, 37, 57 1 33 103, 144 103, 144 103, 144 -5 4.19 10-5 2.93 10-5 2.51 10-5 2. 30 63.05 50.09 40.37 78 -6.30 -9.14 -11.33 89 0.83 0.71 0.62
11,40 61,122 2.85 10-5 50.40 -9.10 0.60	10, 37, 55 86, 125 86, 125 1.82 10—5 49.96 —9.09	11, 37, 57 103, 144 2.93 10 ⁻⁵ 50.09 -9.14 0.71
23,39 63,130 3.14 10 ⁻⁵ 52.35 -6.30 0.86	9, 34, 49 76, 124 1.95 10 ⁻⁵ 62.26 -6.28 0.96	11, 37, 57 103, 144 4.19 10 ⁻⁵ 63.05 -6.30 0.83
22, 4C 64, 13C 4.29 10—5 68.78 —2.80 1.59	9, 30, 46 69, 127 2.41 10 ⁻⁵ 81.82 -2.80	11,37,57 103,133 19.17 10-5 83.30 32.78
9, 37 62, 124 6.73 10 ⁻⁵ 107.31 667	8, 28, 46 69, 128 3.56 10-5 104.63 -0.683	$11,37,57 \\ 103,144 \\ 2.09 10^{-4} \\ 108.02 \\ -0.668 \\ -0.657$
$^3S_1^{}$ $^3D_1^{}$	$^3S_1^{}$ $^3D_1^{}$ ϵ_1	351 3D1
p_1, p_2 p_3, p_4 $p_4 = 5$ p_m	p_1, p_2, p_3 p_4, p_5 γ γ β δ m	$p_1, p_2, p_3,$ p_4, p_5 γ^{av} . δ_{av} .
L=5	T=6	$ \begin{array}{c c} L = 6 & p_1, p_2 \\ \text{(average)} & p_4, p_5 \\ \hline \gamma^{av} & \\ \delta_{av} & \\ \end{array} $

CABLE II

Same as Table I for the ¹S₀ phaseshift.

$E_{ m Lab}[MeV] \ \delta_{ m BBS}$		10 52.10	25 45.05	50 35.15	75 27.33	100 20.86	150 10.24	200 1.75	250 5.40
L=2	$\begin{array}{c} p_1 \\ \gamma^{L=2} \\ \delta_m \end{array}$	58 58 8.47 10 ⁻⁴ 8.39 10 ⁻⁴ 49.50 43.51	58 8.39 10 ⁻⁴ 43.51	56 3.56 10 ⁻⁴ 34.28	56 1.42 10 ⁻⁴ 26.64	56 1.10 10 ⁻⁴ 20.19	56 1.78 10 ⁻⁴ 9.61	56 2.11 10 ⁻⁴ 1.01	56 1.19 10 ⁻⁴ -6.28
L=3	$p_1, p_2 \\ \gamma^L = 3 \\ \delta_m$	60, 134 1.55 10 ⁻⁴ 49.28	59,137 6.58 10 ⁻⁵ 43.41	58, 142 4.24 10 ⁻⁵ 34.13	57, 151 4.03 10 ⁻⁵ 26.56	57, 147 3.41 10 ⁻⁵ 20.11	57, 141 3.67 10 ⁻⁵ 9.52	57, 141 3.08 10 ⁻⁵ 0.91	57, 150 2.26 10 ⁻⁵ -6.41
L=4	p_1, p_2, p_3 $\gamma^{L=4}$ δ_m	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	38,61,136 2.97 10 ⁻⁵ 43.65	48, 71, 135 1.06 10 ⁻⁵ 34.50	$34, 59, 136$ $38, 61, 136$ $48, 71, 135$ $46, 69, 136$ $45, 69, 136$ $47, 74, 134$ $42, 69, 137$ $44, 71, 137$ 8.36 10^{-5} 2.97 10^{-5} 1.06 10^{-5} 6.21 10^{-6} 4.56 10^{-6} 3.05 10^{-6} 2.67 10^{-6} 2.37 10^{-6} 49.45 43.65 34.50 26.96 20.57 10.08 1.65 -5.52	45, 69, 136 4.56 10 ⁻⁶ 20.57	47, 74, 134 3.05 10 ⁻⁶ 10.08	42, 69, 137 2.67 10 ⁻⁶ 1.65	$44, 71, 137$ $2.37 ext{ } 10^{-6}$ -5.52
L=5	p_1, p_2, p_3, p_4 $\gamma^{L=5}$ δ_m	10,45 72,137 2.31 10 ⁻⁵ 52.03	12, 45 74, 134 1.06 10 ⁻⁵ 44.90	11,45 73,136 6.01 10 ⁻⁶ 35.06	20, 46 74, 136 4.41 10 ⁻⁶ 27.08	26,49 77,136 3.48 10 ⁻⁶ 20.54	28,50 77,136 2.61 10 ⁻⁶ 10.08	30, 51 77, 137 2.15 10 ⁻⁶ 1.65	29, 51 77, 138 1.86 10 ⁻⁶ -5.48
L=5 (average)	 P1, P2 P3, P4 γ^{av} δ_{av} 	21,48 75,136 3.83 10 ⁻⁵ 50.72	21,48 75,136 1.45 10 ⁻⁵ 44.25	21,48 75,136 6.98 10 ⁻⁵ 34.71	21,48 75,136 4.81 10 ⁻⁵ 27.03	21, 48 75, 136 3.79 10 ⁻⁵ 20.59	21,48 75,136 2.85 10 ⁻⁵ 10.07	21, 48 75, 136 2.46 10 ⁻⁵ 1.60	21, 48 75, 136 2.29 10 ⁻⁵ -5.55

TABLE III

Same as Table I for the 3P_0 phaseshift.

$E_{\mathrm{Lab}}[MeV]$		10	25	50	75	100	150	200	250
бввя		3.94	8.33	10.16	8.86	6.35	0.27	-5.93	-11.81
L=2	$ \begin{array}{c} p_1 \\ \gamma^L = 2 \\ \delta_m \end{array} $	62 8.63 10 ⁻³ 3.89	62 62 62 63 63 66 8.63 10 ⁻³ 7.61 10 ⁻³ 5.82 10 ⁻³ 4.68 10 ⁻³ 3.41 10 ⁻³ 3.83 10 ⁻³ 3.89 8.15 9.77 8.26 5.53 -1.03	62 5.82 10 ⁻³ 9.77	62 4.68 10 ⁻³ 8.26	63 3.41 10 ⁻⁸ 5.53		78 6.83 10 ⁻³ -7.84	82 1.30 10 ⁻² -13.93
L=3	p_1, p_2 $\gamma^{L=3}$ δ_m	33,61 2.29 10 ⁻³ 3.92	33, 61 1.96 10 ⁻³ 8.28	$34,62 \\ 1.44 10^{-3} \\ 10.11$	34, 62 34, 62 34, 62 33, 62 1.44 10 ⁻³ 1.12 10 ⁻³ 9.25 10 ⁻⁴ 6.97 10 ⁻⁴ 10.11 8.80 6.28 0.15	34,62 9.25 10 ⁻⁴ 6.28	33,62 6.97 10 ⁻⁴ 0.15	32, 61 5.77 10 ⁻⁴ -6.09	32,61 5.00 10 ⁻⁴ -12.06
L=4	p_1, p_2, p_3 $\gamma^{L=4}$ δ_m	p_1, p_2, p_3 25, 53, 112 26, 54, 114 28, 56, 111 29, 56, 117 29, 56, 116 29, 56, 115 30, 57, 118 $\gamma^{L=4}$ 1.02 10^{-3} 8.73 10^{-4} 6.47 10^{-4} 5.02 10^{-4} 4.07 10^{-4} 3.01 10^{-4} 2.44 10^{-4} δ_m 3.91 8.25 10.03 8.77 6.23 0.11 -6.11	26, 54, 114 8.73 10 ⁻⁴ 8.25	28, 56, 111 6.47 10 ⁻⁴ 10.03	29, 56, 117 5.02 10 ⁻⁴ 8.77	29, 56, 116 4.07 10 ⁻⁴ 6.23	25, 53, 112 26, 54, 114 28, 56, 111 29, 56, 117 29, 56, 116 29, 56, 115 30, 57, 118 1.02 10 ⁻³ 8.73 10 ⁻⁴ 6.47 10 ⁻⁴ 5.02 10 ⁻⁴ 4.07 10 ⁻⁴ 3.01 10 ⁻⁴ 2.44 10 ⁻⁴ 3.91 8.25 10.03 8.77 6.23 0.11 -6.11	30, 57, 118 2.44 10 ⁻⁴ -6.11	30, 57, 117 2.09 10 ⁻⁴ -12.04
L=5	p_1, p_2, p_3, p_4 $\gamma^{L=5}$ L=5	27,53 107,177 4.43 10 ⁻⁴ 3.92	28,54 109,180 3.71 10 ⁻⁴ 8.27	29,55 110,181 2.69 10-4 10.08	30,55 108,179 2.06 10 ⁻⁴ 8.79	30,55 107,177 1.68 10-4 6.28	30,55 106,176 1.24 10-4 0.18	30,55 106,177 1.01 10 ⁻⁴ 8.72 -6.06	$30,55$ $105,176$ $8.72 - 10^{-5}$ -11.97
L=5 (average)	P1, P2 P3, P4 γ ^{av.} δ _{av.}	29, 54 106, 177 4.57 10 ⁻⁴ 3.92	29, 54 106, 177 3.75 10 ⁻⁴ 8.28	29, 54 106, 177 2.71 10 ⁻⁴ 10.09	29, 54 106, 177 2.08 10 ⁻⁴ 8.78	29, 54 106, 177 1.71 10 ⁻⁴ 6.26	29, 54 106, 177 1.28 10 ⁻⁴ 0.16	29, 54 106, 177 1.05 10-4 -6.08	29, 54 106, 177 9.15 10 ⁻⁵ -12.00

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