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Evaluation of operator Padé approximants for perturbative expansions in scattering theory

J. Fleischer and M. Pindor*
Department of Theoretical Physics, University of Bielefeld, Bielefeld, Germany
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Considering scattering amplitudes as integral operators, the formal summation of their perturbation expansions can be done using operator Padé approximants. The lowest-order approximant can be considered a natural improvement of the Bethe-Salpeter equation in ladder approximation if one includes one-loop diagrams other than the direct box graph. The problem of how to evaluate the approximants arises. Variational principles for their calculation have been proposed earlier but yielded ambiguous results. A new variational technique, the method of the variational gradient, is presented which provides a unique though elaborate procedure. The applicability of the method is demonstrated in two cases: a simple potential model and the Bethe-Salpeter equation in ladder approximation for nucleon-nucleon scattering.

I. INTRODUCTION

Various forms of Padé approximants have been introduced as tools for the summation of divergent power series.[1] Their applicability to the summation of perturbation theory for two-particle-scattering problems has been tested in the Schrödinger potential theory[2-5] and in the framework of the Bethe-Salpeter equation (BSE).[6-10] In the present work we are particularly concerned with the summation of perturbation expansions in lowest possible order, i.e., using only the first two terms of the (in general strongly divergent) expansion. These correspond in field theory to one-loop approximations and only these can be calculated with a manageable amount of (computer) time.

The method introduced here was first proposed in Ref. 11. It is based on a variational principle for a non-negative functional, which yields optimal values of the off-shell momenta for an operator Padé approximation (OPA).[1,12] Since one is looking for the absolute minimum of the above functional, the method does not have the ambiguities usually involved in variational operator Padé approximants (VOPA).[10,13,14]

This new technique, called the method of the variational gradient (MVG) is presented in detail in Sec. II. Basically, it is a method to find (approximate) matrix elements of the inverse of a linear operator. Therefore the method may have wider applicability than the description of scattering processes.

In Sec. III we show how the method works for potential scattering. We numerically calculate $l=0$ phase shifts for a two-step potential and compare our results with those of Benofy, Gammel, and Mery.[13]

In Sec. IV we apply the method to the BSE for NN scattering with one-boson exchange.[10] Our results for the $^1S_0$ and $^3P_0$ phase shifts are excellent. For the $^3S_1$ we were unable to perform the search for a minimum of our functional since some integrands were changing more rapidly than in the above two cases and the computer time for their integration became so large that a variation was impossible. Although this is not in principle an obstacle it is clear that the MVG cannot be considered as a substitute for solving the BSE with scalar Padé approximants. It was our aim to find a general method which provides as much information as possible from a one-loop approximation.

II. THE METHOD OF THE VARIATIONAL GRADIENT

We consider a linear operator T in a Hilbert space $\mathcal{H}$, which has a formal power-series expansion (with the expansion parameter set equal to 1)

$$T=T_0+T_1+T_2+\cdots . \tag{1}$$

For convenience we assume that T and the T_i $(i=0,1,\ldots)$ are symmetric. The following considerations apply also with minor modifications to the case when T is nonsymmetric. In later applications, however, we consider only the perturbation expansion for the (symmetric) K matrix. From the first two terms we can form the following operator Padé approximant[1]:

$$T_{\mathrm{OPA}}=T_0\frac{1}{T_0-T_1}T_0 . \tag{2}$$

Here, as in the following, we do not consider existence problems. We shall assume that all operations we perform can be defined in a strict mathematical sense. More general conditions will be discussed at the end of this section. Our task will be to develop an approximation method for the calculation of certain matrix elements of T_{OPA}. The starting point for this is the Schwinger

variational principle,[15] which states that the unique stationary value of the functional

$$R_{\alpha\beta}(\psi,\psi') = \langle\psi'|\, T_0\,|\beta\rangle + \langle\alpha|\, T_0\,|\psi\rangle - \langle\psi'|\, T_0 - T_1\,|\psi\rangle\,, \tag{3}$$

with respect to any variations of the states $|\psi\rangle$ and $|\psi'\rangle$, is given by the matrix element of T_{OPA} between the states $|\alpha\rangle$ and $|\beta\rangle$:

$$T^{\alpha\beta}_{\mathrm{OPA}} = \langle\alpha|\, T_{\mathrm{OPA}}\,|\beta\rangle\,. \tag{4}$$

Varying $R_{\alpha\beta}(\psi,\psi')$ with respect to $|\psi\rangle$ and $|\psi'\rangle$ independently gives for their values at which $R_{\alpha\beta}$ becomes stationary the following expressions:

$$|\psi\rangle_{\mathrm{st}} = \frac{1}{T_0 - T_1}\, T_0|\beta\rangle \text{ and } |\psi'\rangle_{\mathrm{st}} = \frac{1}{T_0 - T_1}\, T_0|\alpha\rangle\,. \tag{5}$$

Inserting these into $R_{\alpha\beta}(\psi,\psi')$ yields $T^{\alpha\beta}_{\mathrm{OPA}}$.

In actual calculations the variations with respect to ψ and ψ' are usually performed in two steps. At first one confines oneself, for practical reasons, to a finite-dimensional subspace of $\mathcal{H}$, given by some projection operator P_L:

$$\mathcal{H}_L = P_L\mathcal{H}\,, \quad P_L{}^2 = P_L \tag{6}$$

and spanned by some states $|\varphi_1\rangle = |\alpha\rangle$, $|\varphi_2\rangle = |\beta\rangle$, $|\varphi_3\rangle, \ldots, |\varphi_L\rangle$. It has been shown[16] that the stationary value of $R_{\alpha\beta}$ obtained with $|\psi\rangle$ and $|\psi'\rangle$ varying in $\mathcal{H}_L$ only is given by the OPA evaluated on this subspace, i.e.,

$$\underset{|\psi\rangle,\,|\psi'\rangle\in\mathcal{H}_L}{\text{stat value}} R_{\alpha\beta}(\psi,\psi') = \langle\alpha|\, T_0 P_L\, \frac{1}{P_L(T_0 - T_1)P_L}\, P_L T_0|\beta\rangle \equiv R^L_{\alpha\beta}(\varphi_3,\ldots,\varphi_L)\,. \tag{7}$$

The second step is to vary for a given L the $|\varphi_i\rangle$'s and look for stationary values of $R^L_{\alpha\beta}(\varphi_3,\ldots,\varphi_L)$ (see Refs. 13 and 17). This is called the "variational" OPA (VOPA). It has been shown[17] that if the $|\varphi_i\rangle$'s are chosen such that $|\psi\rangle_{\mathrm{st}}$ and $|\psi'\rangle_{\mathrm{st}}$ of (5) belong to $\mathcal{H}_L$, then $R^L_{\alpha\beta}$ is stationary and equal to $T^{\alpha\beta}_{\mathrm{OPA}}$. The problem, however, is that $R^L_{\alpha\beta}$ may have, in general, many stationary points and one has to select the proper one. To investigate this problem, we analyze $R^L_{\alpha\beta}$ in detail.

The $|\varphi_i\rangle$'s are varied as follows:

$$|\varphi_i\rangle = |\varphi_i^0\rangle + \epsilon\,\delta_{ik}|\chi\rangle \quad (i = 1,\ldots,L;\ k = 3,\ldots,L) \tag{8}$$

with ϵ an infinitesimal parameter, δ_{ik} the Kronecker symbol and $|\chi\rangle$ an arbitrary vector, $|\chi\rangle\in\mathcal{H}$. Then

$$R^L_{\alpha\beta}(\varphi_3,\ldots,\varphi_L) = R^L_{\alpha\beta}(\varphi_3^0,\ldots,\varphi_L^0\rangle + \epsilon r_{\alpha\beta,k}(\chi) + O(\epsilon^2)\,. \tag{9}$$

$R^L_{\alpha\beta}$ is stationary for $|\varphi_i\rangle = |\varphi_i^0\rangle$ if

$$r_{\alpha\beta,k}(\chi) \equiv 0 \tag{10}$$

for all $|\chi\rangle\in\mathcal{H}$. To evaluate $r_{\alpha\beta,k}$, we need the expansion for P_L:

$$P_L(\varphi_1,\ldots,\varphi_L) = P_L(\varphi_1^0,\ldots,\varphi_L^0) + \epsilon\pi(\chi)\,. \tag{11}$$

The operator $\pi(\chi)$ is calculated starting from the following explicit representation of P_L:

$$P_L = \sum_{i,k=1}^{L} |\varphi_i\rangle F^{-1}{}_{ik}\langle\varphi_k|\,, \tag{12}$$

where $F^{-1}{}_{ik}$ is the (i,k) element of the inverse matrix of

$$F_{lm} = \langle\varphi_l|\,\varphi_m\rangle\,. \tag{13}$$

Here we assume the $|\varphi_i\rangle$'s to be linearly independent for F^{-1} to exist but not necessarily orthonormal. We obtain, dropping the superscript zero in $|\varphi_i^0\rangle$:

$$\pi(\chi) = \sum_{i=1}^{L}\left[(I - P_L)|\chi\rangle F^{-1}{}_{ki}\langle\varphi_i| + |\varphi_i\rangle \times F^{-1}{}_{ik}\langle\chi|\,(I - P_L)\right], \tag{14}$$

I being the unity operator in $\mathcal{H}$. Inserting (11) with (14) into (7) finally yields

$$r_{\alpha\beta,k}(\chi) = \langle\alpha k|\,\chi\rangle + \langle\chi|\,\beta k\rangle\,, \tag{15}$$

with

$$\langle\alpha k| = \sum_{i=1}^{L} F^{-1}{}_{ki}\langle\varphi_i|\, \frac{1}{P_L(T_0 - T_1)P_L}\, P_L T_0|\beta\rangle\langle\alpha|\, T_0\left[I - P_L\, \frac{1}{P_L(T_0 - T_1)P_L}\, P_L(T_0 - T_1)\right](I - P_L) \tag{16}$$

and $\langle\beta k|$ obtained from $\langle\alpha k|$ by exchanging $\langle\alpha|$ and $\langle\beta|$. Since (10) is required for any $|\chi\rangle\in\mathcal{H}$, this implies

$$\langle\alpha k| = \langle\beta k| = 0 \text{ for } k = 3, 4, \ldots, L\,, \tag{17}$$

and since $\langle\alpha k|$ factorizes, (17) is fulfilled when either

$$\langle\alpha|\, T_0\left[I - P_L\, \frac{1}{P_L(T_0 - T_1)P_L}\, P_L(T_0 - T_1)\right](I - P_L) = 0 \tag{17a}$$

or

$$c_{k,\beta} \equiv \sum_{i=1}^{L} F^{-1}{}_{ki}\left\langle\varphi_i\right|\frac{1}{P_L(T_0 - T_1)P_L}\, P_L T_0\left|\beta\right\rangle = 0\,. \tag{17b}$$

For convenience we introduce the vector

$$\langle\gamma_\alpha| = \langle\alpha|T_0\left[I - P_L\frac{1}{P_L(T_0-T_1)P_L}P_L(T_0-T_1)\right]. \tag{18}$$

Since $\langle\gamma_\alpha|P_L=0$, we see that in (17a) the factor $(I-P_L)$ is superfluous and (17a) is equivalent to $\langle\gamma_\alpha|=0$ or

$$\langle\alpha|T_0\frac{1}{T_0-T_1} = \langle\alpha|T_0P_L\frac{1}{P_L(T_0-T_1)P_L}P_L, \tag{19}$$

i.e., according to (5) and analogous considerations for $\langle\beta k|$,

$${}_{st}\langle\psi| \ , \ {}_{st}\langle\psi'| \in \mathcal{K}_L . \tag{20}$$

We thus obtain the result that the stationary point of $R^L_{\alpha\beta}$, achieved when $\langle\gamma_\alpha|=0$ and $\langle\gamma_\beta|=0$, coincides with the stationary point of the Schwinger functional and we have

$$R^L_{\alpha\beta} = T^{\alpha\beta}_{\mathrm{OPA}}, \tag{21}$$

what we are looking for. Indeed, this latter relation is obviously true if only $\langle\gamma_\alpha|=0$ *or* $\langle\gamma_\beta|=0$.

The second equation (17b), is explored as follows. Since

$$\frac{1}{P_L(T_0-T_1)P_L}P_LT_0|\beta\rangle \in \mathcal{K}_L . \tag{22}$$

We can write

$$\frac{1}{P_L(T_0-T_1)P_L}P_LT_0|\beta\rangle = \sum_{j=1}^{L} b_j|\varphi_j\rangle . \tag{23}$$

Insertion into (17b) yields

$$\sum_{i,j}^{L} F^{-1}{}_{ki}F_{ij}b_j = \sum_j \delta_{kj}b_j = b_k = 0 \text{ for } k=3,\ldots,L . \tag{24}$$

Thus we have

$$P_LT_0|\beta\rangle = P_L(T_0-T_1)[b_\alpha|\alpha\rangle + b_\beta|\beta\rangle], \tag{25}$$

which means

$$|\psi_\beta\rangle \equiv (T_0-T_1)[b_\alpha|\alpha\rangle + b_\beta|\beta\rangle] - T_0|\beta\rangle \tag{26}$$

is orthogonal to $\mathcal{K}_L$. Since then it is also orthogonal to $|\alpha\rangle$ and $|\beta\rangle$, the coefficients b_α and b_β are determined by a system of two linear equations (provided its determinant is $\neq 0$). $|\psi_\beta\rangle$ being a fixed vector, we see that it is easy to fulfill (17b): for all $|\varphi_i\rangle$'s $\perp |\psi_\beta\rangle$ we have a stationary point of $R^L_{\alpha\beta}$ and it can be shown that the value of $R^L_{\alpha\beta}$ at this stationary point is in general different from $T^{\alpha\beta}_{\mathrm{OPA}}$. Owing to (23) and (24),

$$R^L_{\alpha\beta} = b_\alpha\langle\alpha|T_0|\alpha\rangle + b_\beta\langle\alpha|T_0|\beta\rangle \tag{27}$$

and from (26) we obtain

$$T^{\alpha\beta}_{\mathrm{OPA}} = \left\langle\alpha\left|T_0\frac{1}{T_0-T_1}T_0\right|\beta\right\rangle = b_\alpha\langle\alpha|T_0|\alpha\rangle + b_\beta\langle\alpha|T_0|\beta\rangle - \left\langle\alpha\left|T_0\frac{1}{T_0-T_1}\right|\psi_\beta\right\rangle . \tag{28}$$

Equations (27) and (28) do only agree if ${}_{st}\langle\psi'|\psi_\beta\rangle = 0$, which can never be checked and will not be true in general.

It is interesting to note that, evaluating (27) a bit further, one obtains

$$R^L_{\alpha\beta} = R^2_{\alpha\beta}, \tag{29}$$

i.e., the matrix Padé approximation in the space $\langle\alpha|$, $\langle\beta|$ and in the case $\langle\alpha|=\langle\beta|$ it is just the ordinary scalar approximant. This has been found numerically in Ref. 13.

From the above discussion we have seen that $R^L_{\alpha\beta}$ has two stationary values if we perform the variation over the full $\mathcal{K}$ and only one of them is what we are looking for. In any practical calculation, however, one will parametrize the basis states somehow and do the variation by changing the parameters over a finite region. Varying p, e.g., the infinitesimal change of the $|\varphi_k\rangle$'s will be

$$|\varphi_i(p)\rangle = |\varphi_i(p_0)\rangle + (p-p_0)\,\delta_{ik}|\varphi_i'(p_0)\rangle , \tag{30}$$

i.e., in (8) $|\chi\rangle$ is to be replaced by $|\varphi_k'(p_0)\rangle$. As a result, Eq. (15) reads now

$$r_{\alpha\beta,k} = \langle\alpha k|\varphi_k'(p_0)\rangle + \langle\varphi_k'(p_0)|\beta k\rangle . \tag{31}$$

In contrast to (15), where $|\chi\rangle$ varies over the full $\mathcal{K}$, in (31) the variations are restricted to certain trajectories. Owing to this restriction we find stationary points which can be different from those obtained for $|\gamma_\alpha\rangle=0$ or $|\gamma_\beta\rangle=0$. One possibility is that for a particular $p=p_0$ the above two terms cancel if $\langle\alpha|\neq\langle\beta|$, another that both terms vanish. For $\langle\alpha|=\langle\beta|$ we may have

$$\langle\varphi_k'(p_0)|\gamma_\alpha\rangle = 0 , \tag{32}$$

which can be obtained if we are close to the correct stationary point where $\langle\gamma_\alpha|=0$. Since $\langle\gamma_\alpha|$ is [apart from the coefficient $c_{k,\beta}$ defined in (17b)] the "gradient" of the functional $R^L_{\alpha\beta}$, its direction changes rapidly near the correct stationary point. Considering $|\varphi_k'(p)\rangle$ as nearly constant for $p\simeq p_0$, then (32) can be easily fulfilled and this explains the success of the VOPA's so far. Of course, this condition can accidentally be fulfilled in other regions of the parameters, where the values of $R_{\alpha\beta}$ may have no relation to $T^{\alpha\beta}_{\mathrm{OPA}}$.

According to the above, the only accurate procedure for finding the proper value of $T^{\alpha\beta}_{\mathrm{OPA}}$ is to evaluate the OPA for such $\langle\varphi_i|$'s $\in\mathcal{K}$ which yield $\langle\gamma_\alpha|=0$ or $\langle\gamma_\beta|=0$. Since in practice the variation

performed by changing the parameters of some $|\varphi_i\rangle$'s will in general not yield these vectors, we propose as best approximation to minimize $\langle\gamma_\alpha|\gamma_\alpha\rangle$. This will be superior compared to the search for stationary points of $R^L_{\alpha\beta}$ itself but also more elaborate. We then have a positive functional, the absolute minimum of which yields the best possible values for the parameters in the OPA.

A further interesting relation can be derived by some simple algebra:

$$|R^L_{\alpha\beta}-T^{\alpha\beta}_{\mathrm{OPA}}|=\left|\left\langle\gamma_\alpha\left|\frac{1}{T_0-T_1}\right|\gamma_\beta\right\rangle\right|$$
$$\leq\|\gamma_\alpha\|\times\|\gamma_\beta\|\times\left\|\frac{1}{T_0-T_1}\right\|_{(I-P_L)\mathcal{H}}$$
$$\leq\|\gamma_\alpha\|\times\|\gamma_\beta\|\times\left\|\frac{1}{T_0-T_1}\right\|_{\mathcal{H}}. \qquad (33)$$

Although we have no knowledge of $\|1/T_0-T_1\|$, we see that minimizing $\|\gamma_\alpha\|\times\|\gamma_\beta\|$ can give us reasonable approximations to $T^{\alpha\beta}_{\mathrm{OPA}}$ independently of being close to a stationary point of the functional $R^L_{\alpha\beta}$.

The mathematical condition for the applicability of Eq. (33) is the existence of $\|\gamma_\alpha\|$ and $\|\gamma_\beta\|$, i.e., $\langle\alpha|$ and $\langle\beta|$ belonging to the domain of

$$T_0-(T_0-T_1)P_L\frac{1}{P_L(T_0-T_1)P_L}P_LT_0. \qquad (34)$$

This is much less stringent than what was needed for the study of the variational properties of $R^L_{\alpha\beta}$. The existence of $\|\gamma_{\alpha,\beta}\|$ requires only the existence of the matrix elements $\langle\varphi_i|T_0^2|\varphi_k\rangle$, $\langle\varphi_i|T_0(T_0-T_1)|\varphi_k\rangle$ and $\langle\varphi_i|(T_0-T_1)^2|\varphi_k\rangle$ and these can have meaning even if the $|\varphi_k\rangle$'s do not belong to the domains of T_0^2, T_0T_1, and T_1^2.

If $|\gamma_\alpha\rangle$ or $|\gamma_\beta\rangle$ are not normalizable, there is still the possibility of introducing an operator O into the right-hand side of (33), such that $O|\gamma_{\alpha,\beta}\rangle$ belongs to $\mathcal{H}$ and that $O^{-1}[1/(T_0-T_1)]O^{-1}$ is bounded. We shall not discuss this case here but refer to Ref. 11, where this trick was used.

Finally, we mention how the method can be extended to higher orders. For all OPA's which can be put in the form $AB^{-1}C$, where only positive powers of the T_i's appear in A, B, and C, the Schwinger functional reads

$$R_{\alpha,\beta}(\psi,\psi')=\langle\psi'|C|\beta\rangle+\langle\alpha|A|\psi\rangle-\langle\psi'|B|\psi\rangle \qquad (35)$$

and the method for calculating corresponding matrix elements works as before. For the next higher order, e.g., the OPA reads

$$T^{(2)}_{\mathrm{OPA}}=T_0+T_1\frac{1}{T_1-T_2}T_1 \qquad (36)$$

and the method has to be applied to the second term only.

Similar considerations could be applied to the computation of eigenvalues of symmetric operators. Since, however, there is no ambiguity in a variational solution of the problem (Ref. 17, theorem XII; also Ref. 18), they do not seem necessary.

Finally we mention that a relation analogous to (33) has been proven earlier, though under much more stringent conditions, both for scattering and for bound-state problems.[19,20]

III. APPLICATION TO POTENTIAL SCATTERING

Let us consider the scattering of particles described by the Schrödinger equation with a central potential $V(r)$. The phase shifts can be found from the K matrix:

$$\langle p_\alpha, l|K(E)|p_\beta, l\rangle=\frac{1}{2mp}\tan\delta_l(E), \qquad (37)$$

with $p_\alpha=p_\beta=p$ and $E=p^2/2m$. K is the solution of

$$K(E)=V+VG_0^P(E)K(E) \qquad (38)$$

and G_0^P the principal-value Green's function

$$G_0^P(E)=\tfrac{1}{2}[E-H_0+i\epsilon)^{-1}+(E-H_0-i\epsilon)^{-1}]. \qquad (39)$$

The full solution of (38),

$$K(E)=V\frac{1}{V-VG_0V}V, \qquad (40)$$

is the [1/1] OPA to the Born series corresponding to (38). The MVG allows us to evaluate matrix elements of this approximant by exploiting information contained in the off-shell matrix elements of the perturbation terms.

As in Ref. 13, we calculate S-wave scattering from the potential

$$V(r)=V_1\vartheta(r_1-r)+V_2\vartheta(r_2-r), \qquad (41)$$

where V_1 and V_2 are constants and ϑ is the step function.

Using one off-shell momentum as variational parameter, the above authors have shown (for many values of $V_{1,2}$ and $r_{1,2}$) that one stationary point of the phase shift agreed very accurately with its exact value (Fig. 1 of Ref. 13). They also observed that the phase shift had many other stationary points at the value of the ordinary (scalar) Padé approximant, which property was explained in Sec. I of the present work. The problem with sign changing potentials, however, is that one has no *a priori* reason to choose one stationary point or another and the results are ambiguous.

The situation changes basically if we minimize $\|\gamma\|$, though we have to calculate terms such as $VG_0^PV^2G_0^PV$ which corresponds to one more iteration. For the same case as discussed above,

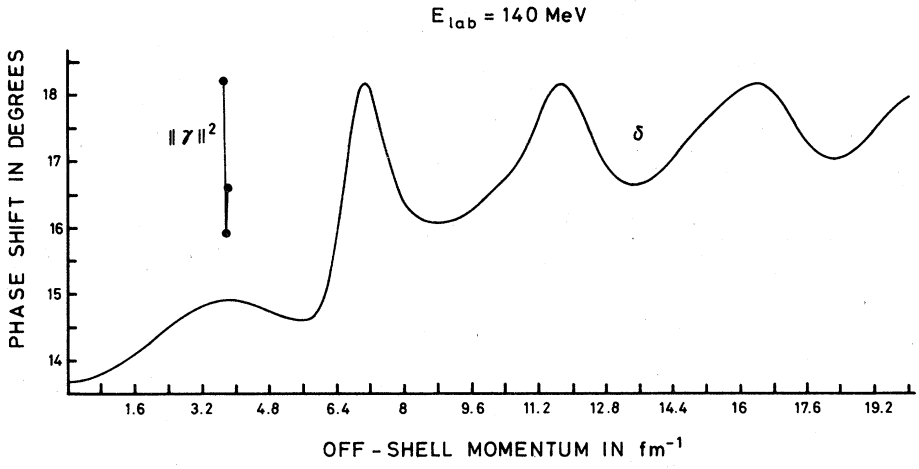

FIG. 1. Dependence of the phaseshift δ on the off-shell momentum at $E_{lab}=140$ MeV. For the potential [see (41)] the parameters are as in Ref. 13 ($V_1=170.05$ MeV, $V_2=-34.01$ MeV, $r_1=0.68$ fm, and $r_2=1.92$ fm). Only three points (see dots) of the $\|\gamma\|^2$ curve (in arbitrary normalization) appear in this figure and are connected by straight lines. The minimum of $\|\gamma\|^2$ is obtained at the off-shell momentum $k_m=3.758$ fm^{-1}. The value of the phase shift at this point is 14.9156° to be compared with the exact value of 14.9174° and the value at the first maximum of 14.9167°.

the minimum of $\|\gamma\|$ points very close to the first maximum as is shown in Fig. 1. For a much stronger potential, however, there is no stationary point of the phase shift near the correct value though the minimum of $\|\gamma\|$ points at a quite reasonable value [see Fig. 2; $p=0$ is an artificial stationary point independent of the energy because we took $\langle r|p,1=0\rangle=\sin pr/p$ and therefore $\delta(p,E)$ and $\|\gamma(p,E)\|$ are even in p]. More details about the results for this potential are given in Table I. As one could expect, increasing the number of the off-shell momenta (i.e., the number of variational vectors $|\phi_i\rangle$) decreases the achieved minimal value of $\|\gamma\|$ and increases the accuracy of the phase shift.

For energies close to values where the phase shift goes through odd multiples of $\pi/2$ (for the above potential this is the case for $E=18.8$) our method does not work very well with only one off-shell momentum as variational parameter. Although there is a minimum of $\|\gamma\|$ pointing to a quite accurate value of the phase shift, there is in general another, comparable or even deeper, minimum at some wrong place and the value of

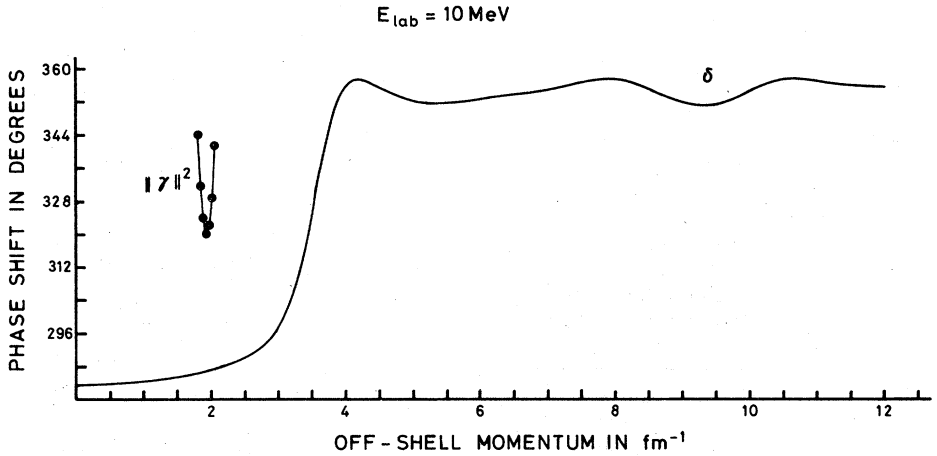

FIG. 2. Same as Fig. 1 for $V_1=1000$ MeV, $V_2=-100$ MeV, $r_1=1$ fm, $r_2=2$ fm, and $E_{lab}=10$ MeV. For these values of the parameters there exist two bound states, i.e., $\delta(E_{lab}=0)=360°$. The minimum of $\|\gamma\|^2$ is obtained at $k_m=1.928$ fm^{-1}. The value of the phase shift at this point is 287.05°, to be compared with the exact value of 289.34°. For two off-shell momenta the phase shift at the minimum of $\|\gamma\|^2$ is 289.26°.

TABLE I. Rate of convergence for the values of the phaseshifts δ_m, obtained at the minimal values of $||\gamma||^2 = \gamma_m^L$, with increasing number of off-shell momenta ($L-1$). $L-1=\infty$ stands for the exact solution and $L-1=0$ for the scalar Padé approximation. E is the energy. The values of the phase shifts are taken within $(-\pi/2, +\pi/2)$. The potential parameters are the same as for Fig. 2.

$L-1$ \ E (MeV)	14.5		100		200		1000	
	δ_m	γ_m^L	δ_m	γ_m^L	δ_m	γ_m^L	δ_m	γ_m^L
1	−83.7	89 000	19.3369	319	−20.1400	230	40.7145	510
2	−81.776	2850	21.2234	21	−18.2820	15	50.3111	46
3	−81.7136	435	21.2772	3.1	−18.2250	2.1	50.6031	5.3
4	−81.7033	103	21.2845	0.76	−18.2186	0.52	50.6111	1.6
5	−81.7022	38	21.2854	0.27	−18.2175	0.18	50.6177	0.46
6					−18.2171	0.074		
∞	−81.7013		21.2860		−18.2169		50.6190	
0	−3.498		−26.84		−52.76		81.57	

$||\gamma||$ at the absolute minimum is extraordinarily large. As is also shown in Table I, increasing the number of off-shell points improves the situation considerably.

It is interesting to note that the values of the off-shell momenta at which $||\gamma||$ achieves a minimum change very little with the energy. This is demonstrated in Table II. When we looked for the phase shift as a function of the energy, we could therefore use the values of the off-shell momenta found for one energy as a very good first guess for the minimizing of $||\gamma||$ at the next energy. An exception occurs again when the phase shift is close to a multiple of $\pi/2$ (see $E=20$ in Table II).

Finally we present in Fig. 3 the comparison of the energy dependence of the exact phase shift with phase shifts obtained from the scalar Padé approximant and through $||\gamma||$ minimization with one and two off-shell momenta. The results are very promising and in the next section we apply the method to a realistic physical model which reproduces the experimental phase shifts.

IV. APPLICATION TO THE BETHE-SALPETER EQUATION FOR *NN* SCATTERING

The Bethe-Salpeter equation (BSE) for *NN* scattering was treated extensively in Refs. 8–10. The *NN* force ("potential") was taken as exchange of π, ρ, ω, ϵ, η, and δ mesons. A cut off was introduced as a form factor at the vertices in order to suppress high-momentum divergences. Taking into account couplings of various spin states and positive and negative energy states, the BSE in momentum space is in general a system of eight coupled integral equations in two variables (relative energy and modulus of three-momentum). It reads

$$\Phi(p, p_0, \alpha) = G(p, p_0, \alpha; \hat{p}, 0, \kappa) - \frac{i}{2\pi^2} \int dq\, dq_0 \sum_{\beta,\gamma} G(p, p_0, \alpha; q, q_0, \beta) S(q, q_0, \beta, \gamma) \Phi(q, q_0, \gamma), \tag{42}$$

with $\hat{p} = (E^2 - m^2)^{1/2}$ (m the nucleon mass) and $\alpha, \beta, \gamma = 1, 2, \ldots, 8$; $\kappa = 1, 2$. For the meaning of labels $1, \ldots, 8$ see Ref. 21. In Eq. (42) G is the kernel and S the two-nucleon propagator. This equation can be solved by iteration and the application of ordinary scalar Padé approximants (up to [5/5], see Refs. 8–10).

Beyond that, various forms of Padé approximants were tested to obtain the solution in a lower order. As one of these methods, the variational

TABLE II. Dependence of the values of the off-shell momenta at the minimum of $||\gamma||^2$ for one ($L=2$) and two ($L=3$) off-shell momenta, respectively. p_0 is the on-shell momentum. The unit for the momenta is fm^{-1}. The potential parameters are the same as for Fig. 2.

E (MeV)	p_0	$\gamma_m^{L=2}$	p_1	$\gamma_m^{L=3}$	p_1	p_2
10	0.347	1.410×10^{4}	1.928	6.376×10^{2}	2.792	4.872
20	0.431	1.137×10^{5}	1.660	3.354×10^{4}	2.745	4.909
50	0.776	1.150×10^{3}	1.851	7.828×10^{1}	2.747	4.912
100	1.098	3.190×10^{2}	1.854	2.087×10^{1}	2.701	4.953
200	1.552	2.260×10^{2}	1.850	1.476×10^{1}	2.623	5.026
500	2.454	2.372×10^{4}	1.843	7.075×10^{2}	2.445	5.219
1000	3.471	5.096×10^{2}	1.596	4.621×10^{1}	2.267	5.596

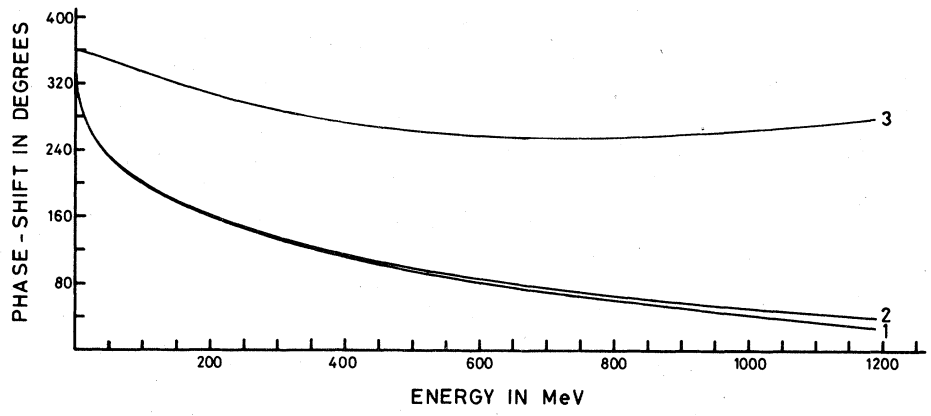

FIG. 3. Energy dependence of the phase shift for various approximants. Curve 1 was obtained with only one off-shell momentum, curve 2 with two and is indistinguishable from the exact curve. Finally, curve 3 is found by using ordinary Padé approximants.

operator Padé approximants (VOPA's),[13,14] were applied, which worked here in a very similar manner as in potential theory. The important problem, however, the question of uniqueness of the variational solution, could not be answered either and only the statement, that the first minimum gives good results in general, could be deduced from the numerical results. The MVG representing a unique procedure, it is worthwhile to investigate its applicability to this case as well. Since the calculation of $\|\gamma\|^2$ requires now a two-dimensional integration (and summation over spin indices) of a complicated function, it is clear at the outset that a search for $\|\gamma\|^2_{\min}$ will be very time consuming.

For the calculation of $\|\gamma\|^2$ we have adopted two different types of integrations: the first for the calculation of $\gamma(q_0, q)$ involves essentially the evaluation of the box graph, for which the same integration procedure was applied as described in Ref. 8. For the integration of

$$\|\gamma\|^2 = \int dq_0 dq\, \gamma^2(q_0, q)\,, \tag{43}$$

because no singularity is present in the area of integration, this integration is simpler and in general does not need as many integration points as the inner integration.

Finally, $\|\gamma\|^2$ depends on the arbitrarily chosen off-shell momenta as variational parameters. Again, each of them is now represented by the relative energy and the modulus of the three-momentum, i.e., we have two variational parameters for each off-shell momentum. This is a further complication. Since, however, the phase shifts are not very sensitive to variations in the relative energy (at least in the case of pseudoscalar pion-nucleon coupling as considered here, cf. also Ref. 10), it is justified to keep it fixed at a small value, as in Ref. 12 for the VOPA. It is taken to be $\hat{p}/8$.

In Tables III and IV we present our results for the $^1S_0$ and $^3P_0$ partial waves. The results were obtained by varying the modulus of the three-momentum. From Table III we see that the $^1S_0$ phase shift is obtained with very high precision using only one off-shell momentum as variational parameter. Similarly the situation is for the $^3P_0$ as long as the phase shift is positive. The negative values of the phase shifts are only badly reproduced with one off-shell momentum. Taking into account a second off-shell momentum, however, improves the situation drastically: the

TABLE III. $^1S_0$ *NN* phase shift for various energies E calculated from one-boson exchange in terms of the Bethe-Salpeter equation ($\delta_{\rm BSE}$) in comparison with the value of the phase shift δ_m, obtained at the off-shell momentum p_1 (in units of the nucleon mass), where $\|\gamma\|^2$ takes its minimal value $\gamma^{L=2}$. Since this off-shell momentum is surprisingly energy independent, we have also calculated the OPA at some energies (indicated by an asterisk) without performing a search for a minimum of $\|\gamma\|^2$. p_0 is the on-shell momentum.

E (MeV)	$p_0=\hat{p}$	$\delta_{\rm BSE}$	δ_m	$\gamma^{L=2}$	p_1
10*	0.073	58.59	57.38	2.403	1.24
25*	0.115	49.37	49.55	0.777	1.24
50	0.163	39.13	39.47	0.327	1.24
100	0.231	24.95	25.38	0.157	1.24
150*	0.283	14.74	14.92	0.114	1.24
200	0.326	6.47	6.45	0.098	1.24
250	0.365	−0.51	−0.75	0.092	1.25

TABLE IV. Same as Table III for $^3P_0$. For energies where the phase shift is negative (200 and 250 MeV), it is necessary to use two off-shell momenta as variational parameters ($L=3$) in order to obtain a good approximation. With the same off-shell moments also the low-energy phase shifts (10 and 25 MeV) are reproduced properly without searching for a minimum of $||\gamma||^2$.

E (MeV)	$p_0=\hat{p}$	δ_{BSE}	δ_m	$\gamma_m^{L=2}$	p_1	$\gamma_m^{L=3}$	p_1	p_2
10*	0.073	4.10	4.06			0.002	0.633	1.44
25*	0.115	8.89	8.80			0.005	0.633	1.44
50	0.163	11.32	11.31	0.011	0.949			
100	0.231	8.33	8.32	0.018	0.859			
150	0.283	2.65	2.46	0.025	0.804			
200	0.326	−3.39	−6.63	0.024	1.14			
200	0.326	−3.39	−3.70			0.011	0.633	1.44
250	0.365	−9.27	−12.62	0.024	1.10			
250	0.365	−9.27	−9.64			0.013	0.639	1.44

value of $||\gamma||^2_{min}$ drops by a factor of ~2 and the phase shift is obtained with good precision.

Concerning the values of p_1 and p_2 where the minimal value of $||\gamma||^2$ is found, they change surprisingly little with the energy—even less than in the previous case of a strong potential (Table II). For some values of the energy (those with an asterisk in Tables III and IV) we therefore present results obtained by merely evaluating the OPA at the indicated off-shell momenta p_1 and p_2, obtained for other energies. The momenta were not varied to minimize $||\gamma||$ but the results for the phase shifts are excellent. This means that the off-shell momenta can be considered to a very good approximation as independent of the energy. Thus, once the off-shell momenta are known, one has a simple representation of the phase shifts for NN scattering in the energy range of elastic scattering.

The most difficult problem, numerically, is the $^3S_1$ phase shift. It turned out that a proper adjustment of the integration mesh in (43) is of extreme importance in this case. The integrand is quite bumpy and therefore a high number of integration points is needed for this integration as well. Therefore the necessary computer time became so large that we were unable to perform a search for $||\gamma||^2_{min}$. For other (renormalizable) field-theoretical models[22] the fast computer code FORMF (Ref. 23) is available for the numerical integration of one-loop integrals and it is our hope that one will be able to perform the necessary integrations in that case with a reasonable amount of computer time. In any case, the obtained results are very promising for the relativistic field theory and the numerical obstacle met in the case of the $^3S_1$ do not appear to be a matter of principle.

V. CONCLUSIONS

The formal summation of a ladder series in terms of an OPA [see T_{OPA} in (2)] is a simple matter. The problem, however, remains how to evaluate this approximant. The straightforward thing to do, namely, to put in more and more off-shell states and observe convergence, works in some cases of the BSE for NN scattering but the method becomes unstable when one includes, e.g., the crossed box graph with pseudoscalar πNN coupling.[10] From the VOPA one can obtain reasonable results also in this case, though not quite unambiguous.[10] The MVG introduced in the present work has no such ambiguities. Since we could show that the method works very well in potential theory and in the case of the BSE, we conclude that we have actually found a proper method to evaluate the OPA, though this method is quite involved.

The approximation (2) is, however, not limited to the case of a ladder series and thus the MVG represents a technique to sum any operator series. Therefore one can proceed and evaluate any field-theoretical model in a complete one-loop approximation with the help of the OPA. The hope is that in such a manner one can achieve a good approximation also in the case of strong interactions. At least the procedure can be considered a natural improvement of the BSE in ladder approximation if one includes one-loop diagrams other than the direct box graphs.

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*At present at the Institute of Theoretical Physics, University of Warsaw, Warsaw, Poland.

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