Variational bounds from matrix Padé approximants in potential scattering

D. Bessis, P. Mery,* and G. Turchetti†

Service de Physique Théorique, Centre d'Etudes Nucleaires de Saclay, BP N° 2-91190 Gif-sur-Yvette, France

(Received 21 December 1976)

We fully develop the content of the Schwinger variational principle for the phase shifts in potential scattering. We introduce matrix Padé approximations built up from the perturbation expansion of the Green's function. They appear to lead to a new type of (Padé) approximation when optimized through the variational principle. These new approximations, which are no longer rational fractions in the expansion parameter, appears to have the full analytical richness of the exact solution. For the case of a nonchanging-sign potential these new types of approximations provide the best bounds to the phase shifts and bound states. The extension to arbitrarily singular potentials is also discussed. A numerical example confirms the extreme efficiency of the method. Typically, for values of the coupling giving rise to one or two bound states the phase shifts are obtained within 10^{-3} of their exact values, and this on the full range of energy, by including only the first and second Born terms of the perturbation series.

INTRODUCTION

Variational methods have been extensively used in potential scattering for computational purposes. Also, Padé approximants (PA's) have been extensively investigated and their convergence properties established for a wide class of potentials.[1-3]

Actually the standard variational procedures have been preferred since they involve almost the same computational difficulties as the second Born approximation and produce very accurate results if the number of trial functions is large enough. The PA's may reach arbitrary accuracy only if an increasingly high number of terms in the Born series is supplied.

However, the algebraic nature of the Padé algorithm finds its full use when a differential or integral equation is lacking and only the perturbation series is available, as in field theory.

Remarkable progress was achieved after realizing that the PA's could be derived from variational principles[4-7] and that the off-shell momenta of the Green's function could be treated as variational parameters.[8] Starting from the Ritz principle the use of PA's on the half-shell T matrix for computing bound states and resonances was rigorously justified.[9] Quite independently, the theory[4,10] and applications[11] of matrix PA's were developed and a great improvement in low-energy nucleon-nucleon scattering was achieved.[12,13] By combining the variational and matrix aspects of the PA's very accurate results were obtained for the phase shifts of a sign-changing potential with a very-low-order approximation.[14] This purely numerical approach was then found to have its theoretical foundation in the Schwinger phase-shift variational principle.[15]

This last approach is the most general since it combines, as we shall prove, the algebraic properties of PA's with the extremal properties in the off-shell momenta. We shall also prove that for potentials of definite sign the phase shifts and bound states computed from the $[N/N]$ PA provide strict bounds, converging monotonically to the exact solution, and that this result can be extended to arbitrarily singular potentials if a suitable regularization procedure is used.[16]

As a numerical example we have considered the S wave for the exponential potentials. The $[1/1]$ PA to the K matrix involving the physical and at most two off-shell momenta always provides very accurate solutions (better than 1%) for coupling far beyond the typical values of strong interactions.

As a consequence the variational matrix PA becomes competitive with the standard variational methods and allows extensions to field-theoretical models to which the standard methods cannot be applied.

I. THE SCHWINGER VARIATIONAL PRINCIPLE FOR PHASE SHIFTS

We consider the scattering operator $K(E)$, the solution of the Lippmann-Schwinger equation, for a Hamiltonian $H = H_0 + gV$,

$$K(E) = gV + gVG_0(E)K(E), \tag{1.1}$$

where

$$G_0(E) = \tfrac{1}{2}[(E + i\epsilon - H_0)^{-1} + (E - i\epsilon - H_0)^{-1}]. \tag{1.2}$$

The formal solution of (1.1) reads

$$K(E) = [1 - gVG_0(E)]^{-1} gV, \tag{1.3}$$

which is the $[1/1]$ operator Padé approximant to $K(E)$.

We assume V to be a positive, regular, central potential and consider a set of eigenstates $|q_\alpha\rangle$ of H_0 and J the total angular momentum (the label j will be omitted); α will take the values $0, 1, \ldots, L-1$ with $E = q_0^2/2m$ and $\mathcal{E}_L$ will be the space spanned by $|q_0\rangle, \ldots, |q_{L-1}\rangle$. The physical amplitude is given by

$$\langle q_0|K(E)|q_0\rangle = -tg\delta/(2mq_0) \tag{1.4}$$

and the off-shell matrix $\mathcal{K}$, restriction of K to $\mathcal{E}_L$, reads

$$\mathcal{K}_{\alpha\beta}(E) = \langle q_\alpha|K(E)|q_\beta\rangle, \quad \alpha,\beta = 0, 1, \ldots, L-1. \tag{1.5}$$

The amplitudes $\mathcal{K}_{\alpha\beta}(E)$ are the stationary values of the Schwinger functionals

$$\mathfrak{K}_{\alpha\beta}(\psi) = g\langle q_\alpha|V|\psi\rangle + g\langle\psi|V|q_\beta\rangle - g\langle\psi|V - gVG_0(E)V|\psi\rangle. \tag{1.6}$$

Letting $\mathcal{E}_L$ be the space spanned by $|q_0\rangle, \ldots, |q_{L-1}\rangle$ and $\mathcal{E}_{LN}$ be the space spanned by

$$(G_0V)^n|q_\alpha\rangle, \tag{1.7}$$
$$n = 0, 1, \ldots, N-1, \quad \alpha = 0, 1, \ldots, L-1$$

it is clear that $\mathcal{E}_{1,L} \subset \mathcal{E}_{2,L} \subset \cdots \subset \mathcal{E}_{N,L} \subset \mathcal{E}$ if $\mathcal{E}$ is the Hilbert space on which K is defined.

The stationary values of $\mathfrak{K}_{\alpha\beta}$, where Ψ varies in $\mathcal{E}_{LN}$, can be worked out and read[15]

$$\mathcal{K}^{LN} = \text{stationary value of } \mathfrak{K}(\Psi)\,|\,\Psi \in \mathcal{E}_{LN}$$
$$= g(\mathcal{K}_1, \ldots, \mathcal{K}_N) \begin{bmatrix} \mathcal{K}_1 - g\mathcal{K}_2 & \cdots & \mathcal{K}_N - g\mathcal{K}_{N+1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \mathcal{K}_N - g\mathcal{K}_{N+1} & \cdots & \mathcal{K}_{2N-1} - g\mathcal{K}_{2N} \end{bmatrix}^{-1} \begin{bmatrix} \mathcal{K}_1 \\ \cdot \\ \cdot \\ \cdot \\ \mathcal{K}_N \end{bmatrix}. \tag{1.8}$$

The meaning of this symbolic notation will be explained in Appendix A, where we also show that $\mathcal{K}^{LN}$ is the $[N/N]$ matrix PA to $\mathcal{K}$.

Consequently we shall write

$$\mathcal{K}^{LN} = [N/N]^L_{\mathcal{K}}, \tag{1.9}$$

where the superscript L has been introduced in order to remind the reader that we deal with $L \times L$ matrices.

The restriction $\mathcal{T}$ of the transition operator T to $\mathcal{E}_L$ is related to $\mathcal{K}$ by

$$\mathcal{T}^{-1} = \mathcal{K}^{-1} + i2mq_0P, \tag{1.10}$$

where $P_{\alpha\beta} = \delta_{\alpha 0}\,\delta_{\beta 0}$ is a projection onto the physical state. Owing to the covariance properties of the matrix PA,[4] Eq. (1.10) is satisfied at any order by the matrix PA to $\mathcal{T}$ and $\mathcal{K}$. As a consequence any convergence property proved for $\mathcal{K}$ will immediately extend to $\mathcal{T}$.

II. VARIATIONAL BOUNDS

If we redefine the vectors in (1.6) so that $|\Psi'\rangle = V^{1/2}|\Psi\rangle$ and $|\phi_\alpha\rangle = V^{1/2}|q_\alpha\rangle$, we then deal with L^2 vectors and a completely continuous operator $V^{1/2}G_0(E)V^{1/2}$. The subspaces $\mathcal{E}_{LN}$ will be defined replacing $|q_\alpha\rangle$ by $|\phi_\alpha\rangle$, and the associated projectors P_{LN} will be introduced.

It is easy to show (see Appendix B) that $\mathcal{K}^{LN}$ is the exact solution of Eq. (1.1) for the potential

$$V_{L,N} = V^{1/2}P_{L,N}V^{1/2}. \tag{2.1}$$

Equation (2.1) gives the physical meaning of the matrix PA.

As a consequence of $\mathcal{E}_{L,N} \subset \mathcal{E}_{L,N+1} \subset \mathcal{E}$ we have

$$V_{L,1} < \cdots < V_{L,N} < V_{L,N+1} < \cdots < V, \tag{2.2}$$

and by the Feynman-Hellman theorem,[17] we get

$$\delta_{L,1} > \cdots > \delta_{L,N} > \delta_{L,N+1} > \delta, \tag{2.3}$$

where $\delta_{L,N}$ is the phase shift corresponding to the on-shell amplitude of $[N/N]^L_{\mathcal{K}}$, that is, the phase shift produced by the potential $V_{L,N}$. This occurs for a given E and $g > 0$. For $g < 0$ the inequalities (2.3) must be reversed.

Similar relations hold if one varies L and N is fixed. Since $\delta_{L,N}$ is obtained from the matrix PA to $\mathcal{K}$, it will depend on the $L-1$ off-shell momenta q_α; as a consequence of (2.3) the best approximation is obtained by choosing the minimum of $\delta_{L,N}$,

$$\min_{\{q_\alpha\}} \delta_{L,N}(E, g, q_1, \ldots, q_{L-1}) \geq \delta(E, g) \tag{2.4}$$

for $g > 0$. For $g < 0$ the min is replaced by max in (2.4) and the inequality is reversed. Equation (2.4) is a very convenient version of the phase-shift variational principle since it is computed from the perturbation series of the Green's function.

Starting from the Ritz principle a similar inequality can be shown to hold for the bound states,[15] namely

$$g_S^{L,N} \leq g_S^{L,N+1} \leq \cdots \leq g_S < 0 \tag{2.5}$$

if g_S labels the value of g for which the Sth bound state occurs at a fixed energy $E<0$.

The computation of the g_S^{LN} is easy since they appear to be the Sth-ordered zeros of the determinant of the matrix PA denominator [i.e., the matrix whose inverse appears in Eq. (1.9)], i.e., the zeros of the Jost function of the potential V_{LN}.[3]

The best approximation is then given by

$$\max_{\{q_\alpha\}} g_S^{LN}(E, g, q_0, q_1, \ldots, q_{L-1}) \leq g_S, \tag{2.6}$$

where also q_0 can be varied since it is no more restricted by the energy-shell condition $q_0^2/2m = E$.

For singular potentials the previous method can be used by introducing a suitable regularization according to the same procedure as for the scalar case.[16] The regularization parameter ϵ then appears as an extra variational parameter.

III. A NUMERICAL EXAMPLE

The variational Padé method has previously been applied for computing the phase shifts and scattering lengths of square-well potentials. For a single square well the exact result is numerically reproduced, using only one off-shell momentum when it is equal to the momentum of the particle inside the well.[18] (Since it is for the semiclassical value of the momentum that the extremum is achieved, we are allowed to think of a deep connection between the variational matrix PA and the WKB method. In fact, it is also conjectured that for a p-wells potential the $[p/p]^{p+1}$ matrix PA provides the exact solution for the physical amplitudes, the extremal values of the off-shell momenta are the classical momenta of the particle in the individual wells.) With two square wells of opposite signs several extrema are found and the extremum closest to the physical momentum always provides a very accurate result.[14] We have considered here a continuous potential in order to have an exhaustive numerical check of the method. The S wave of the exponential potential has been chosen since the analytic solution is known for the S matrix and can be easily worked out up to second order for the off-shell K matrix.

For $V = e^{-\mu r}$ we have computed the phase shifts and scattering lengths for different values of g positive or negative (see Figs. 1–4 and Table I) and the first two bound states $g_n = g_n(E)$ (see Fig. 5). For weak values of g in the attractive case $0 > g \gtrsim -1$ (for $g > -1.44$, there is no bound state so that $g = -1.5$ corresponds roughly to the physical value of the πNN coupling), the results are excellent with a $[1/1]$ PA and $L = 2$, namely when only one off-shell point is used; the exact solution is reproduced within 10^{-3} at any energy. With $L = 3$ the accuracy reaches 10^{-4}. For very high couplings $g \sim -10$ we have two bound states and with $L = 3$ accuracy is still 10^{-2} and rises to 10^{-4} with $L = 5$. For a repulsive interaction the accuracy is always higher for the same value of $|g|$. With $L = 3$ the scattering lengths are reproduced within 10^{-4} for any g. For example, see Fig. 6 for the $[1/1]^L$ matrix PA to the S-wave scattering length for $L = 2, 3$ when $g = 10$.

Finally the first two bound states are reproduced with $L = 2$ within a few percent for $g > -100$. With a sign-changing potential $V = e^{-\mu_1 r} + \rho e^{-\mu_2 r}$, $\rho < 0$,

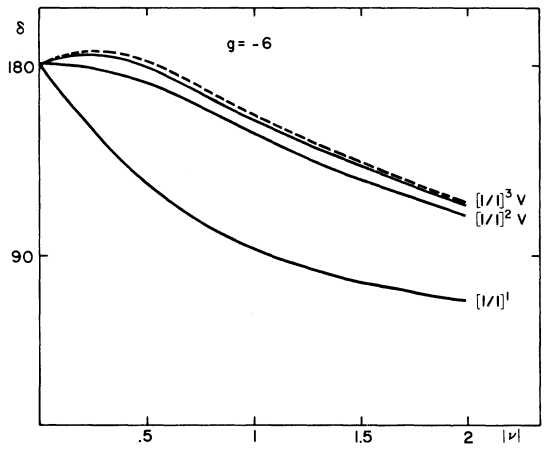

FIG. 1. The exact S-wave phase shift, broken line, of an exponential potential is compared with the scalar $[1/1]^1$ PA and the variational $[1/1]^L$ matrix PA for $L = 2, 3$, namely for one and two off-shell points, for the coupling $g = -6$ in the attractive case. The variables used are defined as in Appendix C.

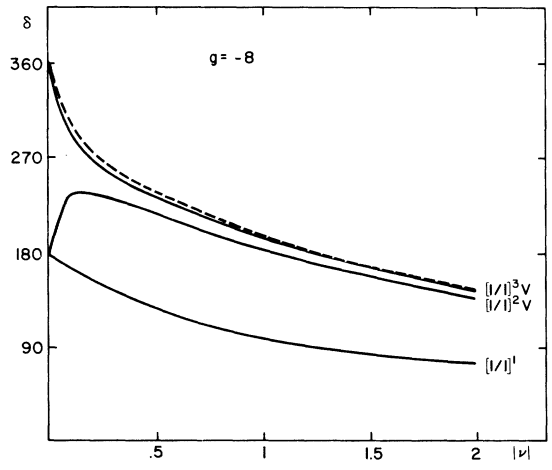

FIG. 2. Same as Fig. 1 but with $g = -8$.

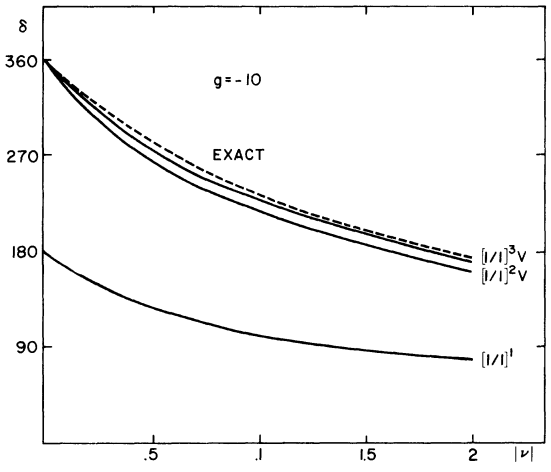

FIG. 3. Same as Fig. 1 but with $g=-10$.

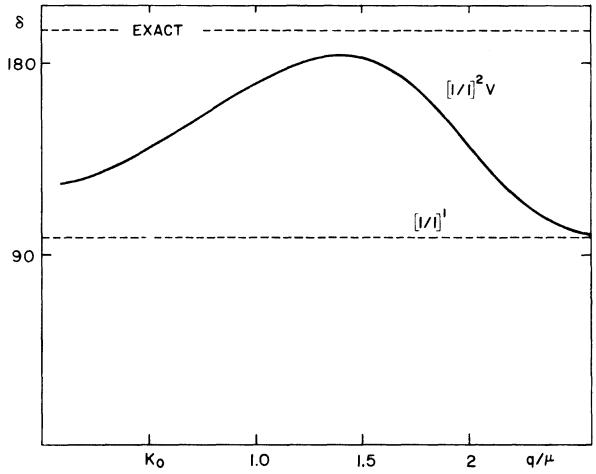

FIG. 4. The variation of the phase shift with the off-shell momentum q_1 is shown for the $[1/1]^2$ matrix PA when $g=-8$, $|\nu|=1$.

the numerical experience shows that if one chooses the extrema corresponding to the values of q_α, which are closest to the physical momentum q_0, usually the phase shift is best reproduced. Furthermore, the accuracy is still comparable to the case where the potential does not change sign even for values of the coupling such that two bound states are present and the phase shift changes its sign. See the particular numerical examples for the sign-changing potential in Figs. 7–9.

IV. CONCLUSION

The method we propose proves to be very efficient and rigorously justified for positive potentials and can be extended to relativistic equations such as the Bethe-Salpeter equations and to many-body nonrelativistic interactions. The method applies to field theory as well since the off-shell Green's function is well defined by its perturbation expansion. Even though the variational procedure cannot be ensured (this may be due to unknown effects of infinite renormalization on the variational principle for the phase shifts), the quasipotential solution[19] will always be provided by the [1/1] matrix PA if the number of off-shell points is increased until numerical stability is reached.

The efficiency of the variational method can be understood if we look at the analytic structure in the coupling constant. The ordinary $[N/N]^L$ matrix PA's are rational functions of g with NL zeros and NL poles; even though infinitely better than a divergent Born series, they can in some cases be

TABLE I. The exact scattering length is compared with the scalar $[1/1]^1$ PA and the variational $[1/1]^L$ matrix PA for $L=2,3$. The extremal values of the off-shell momenta q_1 for $[1/1]^2$ and q_1', q_2' for $[1/1]^3$ are also quoted.

g	Exact	$[1/1]^1$	$[1/1]^2V$	$[1/1]^3V$	q_1/μ	q_1'/μ	q_2'/μ
2.0000	1.8675	1.7778	1.9657	1.8674	0.6240	0.4765	1.1334
4.0000	2.5427	2.2857	2.5398	2.5426	0.5732	0.4246	0.9793
6.0000	2.9465	2.5263	2.9440	2.9465	0.5313	0.3809	0.8459
8.0000	3.2339	2.6667	3.2321	3.2339	0.4957	0.3386	0.7268
10.0000	3.4570	2.7586	3.4558	3.4569	0.4645	0.2782	0.6105
12.0000	3.6393	2.8235	3.6383	3.6388	0.4366	0.1526	0.5105
14.0000	3.7935	2.8718	3.7921	3.7922	0.4114	0.2860	0.4838
16.0000	3.9270	2.9091	3.9247	3.9247	0.3883	0.4130	0.3172
18.0000	4.0448	2.9388	4.0411	4.0418	0.3668	0.6796	0.4285
20.0000	4.1502	2.9630	4.1447	4.1480	0.3466	0.9462	0.4116
22.0000	4.2455	2.9831	4.2377	4.2449	0.3275	1.2128	0.3860
24.0000	4.3325	3.0000	4.3222	4.3323	0.3893	1.3462	0.3691
26.0000	4.4125	3.0145	4.3903	4.4123	0.2918	1.2878	0.3635
28.0000	4.4866	3.0270	4.4703	4.4865	0.2748	1.2544	0.3572
30.0000	4.5556	3.0380	4.5359	4.5555	0.2583	1.2210	0.3520

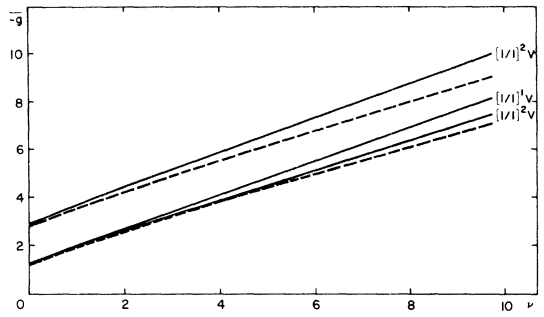

FIG. 5. The exact binding energies for the first and second bound states (broken lines) are compared with the variational $[1/1]^L$ PA for $L=1,2$.

inadequate to approximate the complexity of the analytic structure of the T matrix.

The variational procedure modifies the analytic structure of the PA's, which are no longer rational functions of g. In fact the extremal values of the off-shell momenta are functions of g and allow the PA to get a structure with the same richness of singularities as the exact solution.

The best example of such a mechanism is provided by the $[1/1]^2$ PA for a square well: Before the variational choice of q_1 the $[1/1]^2$ is a rational function with two poles; after that $[1/1]^2$ is the exact solution, namely a function with an infinite number of poles.

APPENDIX A: MATRIX PADÉ APPROXIMANTS

Let $T(x)$ be an analytic matrix with Taylor expansion at the origin given by

$$T(x)=\sum_{k=0}^{\infty} x^k T_k. \tag{A1}$$

The right Padé approximants are defined by

$$^R[N/M]_{T(x)} = {}^RP_N(x)\,{}^RQ_M^{-1}(x) \tag{A2}$$

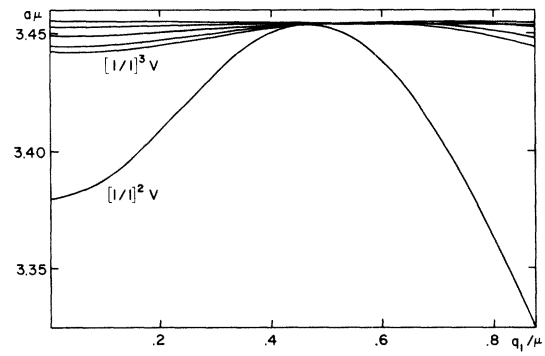

FIG. 6. The $[1/1]^L$ matrix PA to the S-wave scattering length for $L=2,3$ is plotted against the off-shell momentum q_1 when $g=10$. For $[1/1]^3$ the various curves correspond to $q_2/\mu=0.1$, 0.2, 0.3, 0.4, 0.5.

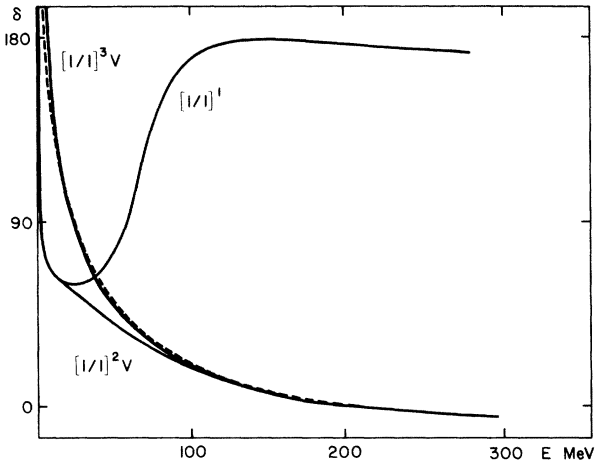

FIG. 7. The exact S-wave phase shift (broken line) for the sign-changing potential $V(r)=V_1\,e^{-r/r_1}+V_2\,e^{-r/r_2}$ is compared with the scalar $[1/1]^1$ PA and the variational $[1/1]^L$ matrix PA for $L=2,3$. We have chosen $V_1=500$ MeV, $V_2=-90$ MeV, $r_1=0.6$ F, $r_2=2.8$ F, and $4m=\hbar=1$ so that $q_0=(E/41.4682)^{1/2}$ F^{-1}, where E is the energy in MeV.

and the left PA's by

$$^L[N/M]_{T(x)} = {}^LQ_M^{-1}(x)\,{}^LP_N(x), \tag{A3}$$

where $^RQ_M(x)$, $^LQ_M(x)$ and $^RP_N(x)$, $^LP_N(x)$ are matrix polynomials of degrees M and N in x, such that

$$T(x)\,{}^RQ_M(x) - {}^RP_N(x) = O(x^{N+M+1}), \tag{A4}$$

$${}^LQ_M(x)T(x) - {}^LP_N(x) = O(x^{N+M+1}). \tag{A5}$$

Theorem I. If the left and right PA's exist they are equal. It is a trivial consequence of the definition. By virtue of this theorem we shall drop the label R or L in $[N/M]$.

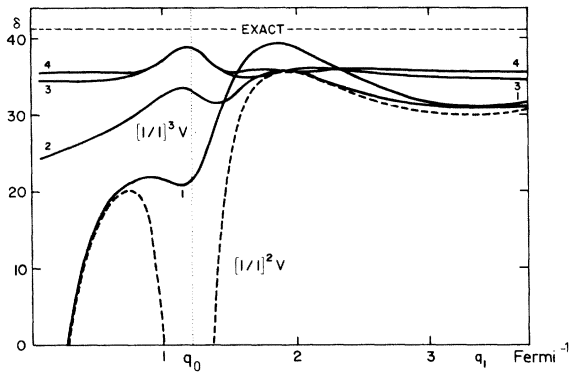

FIG. 8. The phase shifts obtained from the $[1/1]^L$ matrix PA for $L=2,3$ are plotted against the off-shell momentum q_1 for the same potential as in Fig. 7 at $E=60$ MeV. For $[1/1]^3$ the curves 1, 2, 3, 4 correspond to $q_2=1.25$, 1.5, 1.75, 2 F^{-1}, respectively. The exact phase shift is $\delta=41.458$ and the $[1/1]^1$ scalar PA gives $\delta=93.398$.

From (A4) [or (A5)] we get a system of linear equations for the coefficients of ${}^{R}Q_M, {}^{R}P_N$ (${}^{L}Q_M$, ${}^{L}P_N$). Letting

$$ {}^{R}Q_M(x)=\sum_{k=0}^{M}x^k q_k, \qquad {}^{R}P_N(x)=\sum_{k=0}^{N}x^k p_k, \tag{A6} $$

the linear equations read

$$ \sum_{k=0}^{j}T_{j-k}q_k=0, \quad N+1\le j\le N+M \tag{A7} $$

$$ \sum_{k=0}^{j}T_{j-k}q_k=p_j, \quad 0\le j\le N \tag{A8} $$

with the convention $q_k=0$ for $k>M$.

The computation of the PA by solving (A7) is somewhat involved, and we will show that an equivalent symmetric form, more suitable for computational purposes, can be derived using the following variational principles.

The equivalence theorems which state the equality of the right-hand form, the left-hand form, and the symmetric form will be given for $M=N+1$; the generalizations are obvious.

Let $\mathcal{R}$, $\mathcal{L}$, and $\mathcal{H}$ be the functionals

$$ \mathcal{L}=\sum_{i=0}^{N}x^i\lambda_i T_i, \tag{A9} $$

$$ \mathcal{R}=\sum_{i=0}^{N}x^i T_i\mu_i, \tag{A10} $$

$$ \mathcal{H}=\sum_{i=0}^{N}\sum_{k=0}^{N}\lambda_i(T_{i+k}-xT_{i+k+1})\mu_k x^{i+k}, \tag{A11} $$

and define $\mathcal{F}_1$ and $\mathcal{F}_2$ by

$$ \mathcal{F}_1(\lambda,\mu)=\mathcal{L}+\mathcal{R}-\mathcal{H}, \tag{A12} $$

$$ \mathcal{F}_2(\lambda,\mu)=\mathcal{R}\mathcal{H}^{-1}\mathcal{L}. \tag{A13} $$

The stationary value of $\mathcal{F}_1$ is obtained by solving the following linear system in λ and μ:

$$ \frac{\partial\mathcal{F}_1}{\partial\lambda_i}=\frac{\partial\mathcal{L}}{\partial\lambda_i}-\frac{\partial\mathcal{H}}{\partial\lambda_i} =x^i\left[T_i-\sum_{k=0}^{N}(T_{i+k}-xT_{i+k+1})\mu_k x^k\right] =0, \tag{A14} $$

$$ \frac{\partial\mathcal{F}_1}{\partial\mu_i}=\frac{\partial\mathcal{R}}{\partial\mu_i}-\frac{\partial\mathcal{H}}{\partial\mu_i} =x^i\left[T_i-\sum_{k=0}^{N}\lambda_k(T_{i+k}-xT_{i+k+1})x^k\right] =0. \tag{A15} $$

We shall still label by λ_k and μ_k the solutions of (A14) and (A15) and write

$$ \mathcal{L}_{st}=\mathcal{L}(\lambda), \quad \mathcal{R}_{st}=\mathcal{R}(\mu), \quad \mathcal{H}_{st}=\mathcal{H}(\lambda,\mu), \quad \mathcal{F}_1^{st}=\mathcal{L}_{st}+\mathcal{R}_{st}-\mathcal{H}_{st}. \tag{A16} $$

The stationary value of $\mathcal{F}_2$ is obtained from

$$ \frac{\partial\mathcal{F}_2}{\partial\lambda_i}=\mathcal{R}\mathcal{H}^{-1}\frac{\partial\mathcal{L}}{\partial\lambda_i}-\mathcal{R}\mathcal{H}^{-1}\frac{\partial\mathcal{H}}{\partial\lambda_i}\mathcal{H}^{-1}\mathcal{L}=0, \tag{A17} $$

$$ \frac{\partial\mathcal{F}_2}{\partial\mu_i}=\frac{\partial\mathcal{R}}{\partial\mu_i}\mathcal{H}^{-1}\mathcal{L}-\mathcal{R}\mathcal{H}^{-1}\frac{\partial\mathcal{H}}{\partial\mu_i}\mathcal{H}^{-1}\mathcal{L}=0. \tag{A18} $$

We label by λ_k' and μ_k' the solutions of (A17) and (A18), which can be explicitly written as

$$ T_i\,\mathcal{L}_{st}'^{-1}\mathcal{H}_{st}'-\sum_{k=0}^{N}(T_{i+k}-xT_{i+k+1})\mu_k' x^k=0, \tag{A19} $$

$$ \mathcal{H}_{st}'\mathcal{R}_{st}'^{-1}T_i-\sum_{k=0}^{N}\lambda_k'(T_{i+k}-xT_{i+k+1})x^k=0, \tag{A20} $$

where we have set

$$ \mathcal{L}_{st}'=\mathcal{L}(\lambda'), \quad \mathcal{R}_{st}'=\mathcal{R}(\mu'), \quad \mathcal{H}_{st}'=\mathcal{H}(\lambda',\mu'), \quad \mathcal{F}_2^{st}=\mathcal{R}_{st}'\mathcal{H}_{st}'^{-1}\mathcal{L}_{st}'. $$

Theorem II. The stationary values of $\mathcal{F}_1$ and $\mathcal{F}_2$ are identical and one further has

$$ \mathcal{L}_{st}=\mathcal{R}_{st}=\mathcal{H}_{st}=\mathcal{F}_1^{st}=\mathcal{F}_2^{st}. \tag{A21} $$

Left-multiplying (A14) by λ_i and summing over i we get $\mathcal{L}_{st}=\mathcal{H}_{st}$; right-multiplying (A15) by μ_i we get $\mathcal{R}_{st}=\mathcal{H}_{st}$. As a consequence

$$ \mathcal{F}_1^{st}=\mathcal{L}_{st}+\mathcal{R}_{st}-\mathcal{H}_{st}=\mathcal{L}_{st}=\mathcal{R}_{st}=\mathcal{H}_{st}. $$

In order to prove the last part of theorem II we left-multiply (A19) by $\mathcal{H}_{st}'^{-1}\mathcal{L}_{st}'$ and notice that $\mu_k'\mathcal{H}_{st}'^{-1}\mathcal{L}_{st}'$ fulfills the same system of equations as μ_k, namely (A14); consequently we have

$$ \mu_k=\mu_k'\mathcal{H}_{st}'^{-1}\mathcal{L}_{st}'. \tag{A22} $$

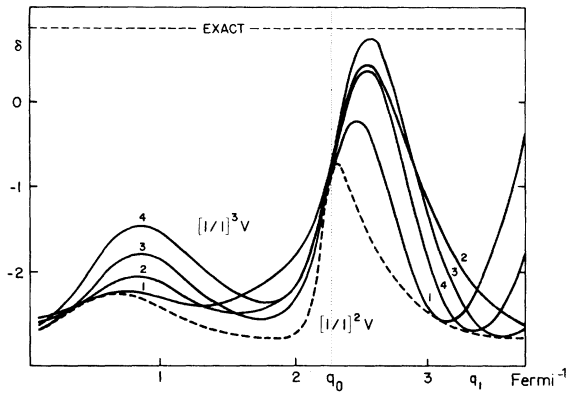

FIG. 9. The same as Fig. 8 for $E=200$ MeV. The exact result is $\delta=0.906$ and the $[1/1]^1$ scalar PA gives $\delta=177.24$.

Right-multiplying (A20) by $\mu_i x^i$ and left-multiplying by $\mathcal{R}'_{st}\mathcal{H}'^{-1}_{st}$ we get, accounting for (A22),

$$\begin{aligned}\mathcal{R}_{st} &= \sum_{i=0}^{N} T_i \mu_i x^i \\ &= \mathcal{R}'_{st}\mathcal{H}'^{-1}_{st} \sum_{i=0}^{N}\sum_{k=0}^{N} \lambda'_k (T_{i+k} - x T_{i+k+1})\mu'_i \\ &\qquad \times x^{i+k}\mathcal{H}'^{-1}_{st}\mathcal{L}'_{st} \\ &= \mathcal{R}'_{st}\mathcal{H}'^{-1}_{st}\mathcal{L}'_{st} \\ &= \mathcal{F}_2^{st}. \end{aligned} \tag{A23}$$

Theorem III. The stationary value of $\mathcal{F}_2$ is the right (or left) $[N/N+1]$ Padé approximant. We notice that Eq. (A19) can be written

$$\sum_{k=0}^{N} q_{N+1-k} T_{i+k} = 0, \quad i = 0, \ldots, N \tag{A24}$$

where

$$\begin{aligned} q_{N+1} &= \mu'_0 - \mathcal{L}'^{-1}_{st}\mathcal{H}'_{st}, \\ q_{N+1-k} &= x^k(\mu'_k - \mu'_{k-1}), \quad k = 1, \ldots, N, \\ q_0 &= -x^{N+1}\mu'_N. \end{aligned} \tag{A25}$$

If we change the indices in (A24) according to $k' = N+1-k$ and $j = N+1+i$ we see that (A24) and (A6) are identical and

$$\begin{aligned} {}^R Q_{N+1}(x) &= \sum_{k=0}^{N+1} x^k q_K \\ &= -x^{N+1}\mathcal{L}'^{-1}_{st}\mathcal{H}'_{st} \end{aligned} \tag{A26}$$

is the denominator of $[N/N+1]$. The last relation in (A26) is obtained accounting for (A25). We notice that (A25) implies

$$\sum_{k=0}^{j} x^k q_k = -x^{N+1}\mu'_{N-j}, \quad j = 0, \ldots, N \tag{A27}$$

and

$$\begin{aligned} -x^{N+1}\mathcal{R}'_{st} &= \sum_{l=0}^{N} x^l T_l(-\mu'_l x^{N+1}) \\ &= \sum_{l=0}^{N}\sum_{k=0}^{N-l} x^{l+k} T_l q_k \\ &= \sum_{j=0}^{N} x^j \sum_{k=0}^{j} T_{j-k} q_k \\ &= {}^R P_N(x), \end{aligned} \tag{A28}$$

where (A8) has been used to identify the numerator of the $[N/N+1]$ PA.

Finally from (A25) and (A28) we get

$$\begin{aligned} \mathcal{F}_2^{st} &= \mathcal{R}'_{st}\mathcal{H}^{-1}_{st}\mathcal{L}'_{st} \\ &= {}^R P_N(x)\, {}^R Q_{N+1}^{-1}(x) \\ &= [N/N+1]_{T(x)}. \end{aligned} \tag{A29}$$

Theorem IV. The symmetric form of the $[N/N+1]$ PA is given by

$$[N/N+1]_{T(z)} = (T_0, T_1, \ldots, T_N) \begin{bmatrix} T_0 - xT_1 & \cdots & T_N - xT_{N+1} \\ \vdots & & \vdots \\ T_N - xT_{N+1} & \cdots & T_{2N} - xT_{2N+1} \end{bmatrix}^{-1} \begin{bmatrix} T_0 \\ T_1 \\ \vdots \\ T_N \end{bmatrix}. \tag{A30}$$

In fact replacing $\lambda_i x^i$ by λ_i and $\mu_k x^k$ by μ^k and setting

$$M_{ik} = T_{i+k} - x T_{i+k+1},$$

we can write

$$\begin{aligned} \mathcal{F}_1 &= \sum_{i=0}^{N}(T_i\mu_i + \lambda_i T_i) - \sum_{i=0}^{N}\sum_{k=0}^{N}\lambda_i M_{ik}\mu_k \\ &= \tilde{T}\mu + \tilde{\lambda}T - \tilde{\lambda}M\mu. \end{aligned} \tag{A31}$$

The stationary condition for $\mathcal{F}_1$ gives

$$\tilde{T} = \tilde{\lambda}M, \quad T = M\mu \tag{A32}$$

and the stationary value of $\mathcal{F}_1$ obtained replacing λ, μ from (A32) in (A31) gives

$$\mathcal{F}_1^{st} = \tilde{T}M^{-1}T. \tag{A33}$$

We recognize that (A33) is the right-hand side of (A30) and by theorems II and III it is the $[N/N+1]$ PA.

In Eq. (A30) we have introduced a block matrix and block vectors; the blocks are the $L \times L$ matrices T_n. Vector matrix multiplication must first be performed according to the standard rules on the individual blocks and then the block products must be computed as $L \times L$ matrix products. The inverse of the block matrix is the actual inverse of an $L(N+1)\times L(N+1)$ matrix and will be cast in a block structure itself.

APPENDIX B

It can be shown that the variational solution (1.9) is identical to the exact resolvent of $P_{LN}V^{1/2}G_0V^{1/2}P_{LN}$ restricted to the subspace $\mathcal{E}_{N,L}$. Since we have proved that (1.9) is a matrix PA we write

$$([N-1/N]_{\mathcal{K}/g})_{\alpha\beta}=\langle q_\alpha|V^{1/2}[1-gP_{LN}V^{1/2}G_0(E)V^{1/2}P_{LN}]^{-1}V^{1/2}|q_\beta\rangle. \tag{B1}$$

Setting

$$A=P_{LN}V^{1/2}, \tag{B2}$$

$$A^\dagger=V^{1/2}P_{LN}, \tag{B3}$$

$$A^\dagger A=V^{1/2}P_{LN}V^{1/2}=V_{LN}, \tag{B4}$$

and accounting for $P_{LN}V^{1/2}|q_\alpha\rangle=V^{1/2}|q_\alpha\rangle$ we get

$$\begin{aligned}([N-1/N]_{\mathcal{K}/g})_{\alpha\beta}&=\langle q_\alpha|A^\dagger[1-gAG_0(E)A^\dagger]^{-1}A|q_\beta\rangle\\&=\langle q_\alpha|A^\dagger A[1-gG_0(E)A^\dagger A]^{-1}|q_\beta\rangle\\&=\langle q_\alpha|V_{LN}[1-gG_0(E)V_{LN}]^{-1}|q_\beta\rangle\\&=\langle q_\alpha|V_{LN}^{1/2}[1-V_{LN}^{1/2}G_0(E)V_{LN}^{1/2}]^{-1}V_{LN}^{1/2}|q_\beta\rangle,\end{aligned}$$

and it is evident that the $[N-1/N]$ PA is the exact solution for the nonlocal potential V_{LN}.

Furthermore, from a known property of the PA we have

$$[N/N]_{\mathcal{K}}=g[N-1/N]_{\mathcal{K}/g}. \tag{B6}$$

APPENDIX C

Setting $\hbar=1$ our model Hamiltonian $H=H_0+V$ reads

$$H_0=-\frac{1}{2m}\Delta, \quad V(r)=V_0e^{-\mu r}. \tag{C1}$$

The integral equation for the stationary S-wave function $\phi(q,r)$ which vanishes at $r=0$ is given by

$$\phi(q,r)=\frac{\sin qr}{q}-2m\int_0^\infty dr'\frac{\sin q_0r_<}{q_0}\cos q_0r_>\times V(r')\phi(q,r'), \tag{C2}$$

where $r_<=\min(r,r')$, $r_>=\max(r,r')$, and $q_0=(2mE)^{1/2}$. The off-shell K matrix reads

$$\langle q'|K(E)|q\rangle=\int_0^\infty dr\frac{\sin q'r}{q'}V(r)\phi(q,r). \tag{C3}$$

In order to have dimensionless variables we have set

$$\nu=\frac{2}{\mu}(-2mE)^{1/2}, \quad g=\frac{2m}{\mu^2}V_0. \tag{C4}$$

In the scattering region $E>0$ we have

$$\nu=-\frac{2i}{\mu}(2mE)^{1/2}=-\frac{2i}{\mu}q_0. \tag{C5}$$

The S matrix $S=e^{2i\delta_0}$ is given by

$$S=H(-\nu,g)/H(\nu,g), \tag{C6}$$

where

$$H(\nu,g)=1+\sum_{k=1}^\infty\frac{g^k}{k!}\frac{1}{(\nu+1)(\nu+2)\cdots(\nu+k)}. \tag{C7}$$

The off-shell amplitudes computed from (C2) and (C3) explicitly read

$$K_1(q,q')=\frac{1}{2m\mu}\frac{2\mu^2}{\mu^2+(q-q')^2}\frac{\mu^2}{\mu^2+(q+q')^2}, \tag{C8}$$

$$\begin{aligned}K_2(q,q')=&-\frac{1}{2m\mu}\frac{\mu^3}{2q_0qq'}[F(q,q')+F(-q,-q')\\&-F(q,-q')-F(-q,q')]\\&+2m\mu\tfrac{1}{2}\nu K_1(q,q_0)K_1(q_0,q')\theta(-E),\end{aligned} \tag{C9}$$

where

$$\begin{aligned}F(q,q')=&\frac{1}{2}\frac{\mu^2}{\mu^2+(q_0+q)^2}\frac{\mu(2q_0+3q+q')}{4\mu^2+(q+q')^2}\\&+\frac{1}{2}\frac{\mu^2}{\mu^2+(q_0-q)^2}\frac{\mu(q_0+q')}{\mu^2+(q_0+q')^2}.\end{aligned} \tag{C10}$$

For $E<0$, q_0 will be replaced by $i\frac{1}{2}\mu\nu$.

*Present address: Centre de Physique Théorique et Université de Lumini—Marseille, France.
†Present address: Istituto di Fisica della Universita—Bologna, INFN sezione di Bologna, Bologna, Italy.

[1]G. Baker, in *Padé Approximants in Theoretical Physics* edited by G. Baker and J. Gammel (Academic, New York, 1970).
[2]C. R. Garibotti and M. Villani, Nuovo Cimento 59A,

107 (1969).
[3]C. R. Garibotti and M. Villani, Nuovo Cimento 61A, 74 (1969).
[4]D. Bessis, in *Padê Approximants*, P. R. Graves Morris (Institute of Physics, London, 1973).
[5]J. Nuttal, in *Padê Approximants in Theoretical Physics*, edited by G. Baker and J. Gammel (Academic, New York, 1970).
[6]D. Bessis and J. Talman, Rocky Mount. J. Math. 4, 151 (1974).
[7]D. Bessis and M. Pusterla, Nuovo Cimento 54, 243 (1968).
[8]C. Alabiso, P. Butera, and G. M. Prosperi, Lett. Nuovo Cimento 3, 831 (1970).
[9]C. Alabiso, P. Butera, and G. M. Prosperi, Nucl. Phys. B31, 141 (1971); B42, 493 (1972).
[10]J. L. Basdevant, D. Bessis, and J. Zinn-Justin, Nuovo Cimento 60A, 185 (1969), mathematical appendix.
[11]D. Bessis, in *Padê Approximants and Their Application* edited by P. R. Graves-Morris (Academic, New York, 1973); G. Turchetti, *ibid.*
[12]D. Bessis, G. Turchetti, and W. Wortman, Nuovo Cimento 22A, 157 (1974); P. Mery and G. Turchetti, Phys. Rev. D 11, 2000 (1975).
[13]P. Mery, Ph.D. thesis, Université de Lumini, Marseille, 1976 (unpublished).
[14]L. P. Benofy, J. Gammel, and P. Mery, Phys. Rev. D 13, 3111 (1976).
[15]G. Turchetti, Lett. Nuovo Cimento 15, 129 (1976).
[16]D. Bessis, L. Epelé, and M. Villani, J. Math. Phys. 15, 2071 (1974).
[17]R. Sugar and R. Blankenbecler, Phys. Rev. 136, B472 (1964).
[18]F. Ortolani, G. Fratamico, and G. Turchetti, Lett. Nuovo Cimento 17, 582 (1976).
[19]I. T. Todorov, Phys. Rev. D 3, 2351 (1971).