Analytic Sturmian functions and convergence of separable expansions

K. Hartt and P. V. A. Yidana
Physics Department, University of Rhode Island, Kingston, Rhode Island 02881
(Received 21 January 1986)

A method for solving integral equations is developed and applied to the homogeneous Lippmann-Schwinger equation in momentum space. It has been used with Yukawa-type potentials, $V(r)=\sum_{j=1}^{N} V_j[\exp(-\mu_j r)]/(\mu_j r)$, and yields solutions that are analytic expressions rational in the variable k^2. More specifically, the principal-value form of the homogeneous Lippmann-Schwinger equation is solved by making an analytic series expansion of the integral, which is then summed using Padé approximants. An application to the Malfliet-Tjon potential V in s wave is given. In a finite subspace of rational functions with fixed denominators, the solutions, referred to as Sturmian functions, are obtained corresponding to the energy -0.35 MeV, which is the physical bound state energy for this potential. With these analytic eigenfunctions as form factors and with the associated eigenvalues, a separable expansion, namely, the unitary pole expansion, is constructed for the local potential. The unitary pole expansion is then used for analytic k-matrix calculations. At intermediate energies through $E_{\text{c.m.}}=666$ MeV, and at ultrahigh momenta, as the rank of the unitary pole expansion approaches 13, analytic wave functions (or, equivalently, half-shell k matrices) and phase shifts are found that are in good agreement with exact results. This is in accord with our observation that separable expansions should not be regarded as low energy approximations, but instead are finite l approximations, for the following reason. For the class of potentials we consider, the partial wave two-body operators $V_l(p,q)$, $t_l(p,q,E)$, and $k_l(p,q,E)$ are compact even though $V(r)$, $T(\mathbf{p},\mathbf{q},E)$, and $K(\mathbf{p},\mathbf{q},E)$ are not compact. Therefore, in principle, these partial wave operators can be approximated by sequences of separable expansions which converge to them in norm. We show that the unitary pole expansion may be such a sequence. There is a practical need for analytic separable expansions that converge more rapidly. In this light we illustrate how our solutions can be used with the Ernst-Shakin-Thaler formulation of separable expansions, and we also discuss the application of our method to the calculation of Gamow states.

I. INTRODUCTION

Strong interactions are perhaps put in their simplest form with the use of separable expansions of potentials. Such a separable expansion for a two-body potential, for example, may be written

$$V=\sum_{i,j=1}^{N} |g_i\rangle C_{ij}\langle f_j| \ ,$$

where the $|g_i\rangle$ and $\langle f_j|$ are referred to as form factors, N is the rank, and the C_{ij} is a constant matrix when the potential is energy-independent. Because the two-nucleon interaction is so complex[1-3] as to be unwieldy in all applications except the two-body problem, much effort has been devoted to the development of various schemes for making separable expansions (SE). Early demonstrations of the technical simplicity of using separable interactions in nuclear two-body[4] and three-body[5] systems were followed by a host of SE formalisms, many of which have their origins in degenerate kernel approximants of two-body scattering equations.

It is beyond the scope of this paper to dwell on interesting interconnections among these formalisms and their relative merits in achieving convergence.[6] However, we should like to categorize some of the better-known methods. One category includes methods that arise from solving either the Schrödinger or the Lippmann-Schwinger equation and have therefore found their most natural formulations in terms of numerical solutions out of which the form factors are constructed. This includes the Weinberg expansion,[7] the unitary pole approximation (UPA),[8] the unitary pole expansion (UPE),[9] and others,[10] which employ Sturmian functions. In addition, Ernst, Shakin, and Thaler[11] (EST) introduced solutions of the Lippmann-Schwinger equation at an arbitrary discrete set of energies. Numerous other investigations have utilized Gamow states,[12,13] wherein energies are not arbitrary, but are prescribed by resonance, bound-state and antibound-state poles of the S matrix. Other schemes that are iterative are associated with collocation methods[14-16] and the use of continued fractions.[17]

A second category includes methods that emphasize the use of analytic expressions for form factors over numerical solutions.[18-20] It is generally helpful in few-body problems to use form factors given in terms of analytic expressions. This is essentially true when the use of contour deformation techniques is desired.[21] When form factors are given in terms of a set of basis functions, it has been found that a significant degree of basis optimization is possible, in part through appeal to variational principles.[18,19] In the most extensive series of applications to date to NN, N$\bar{\text{N}}$, and πN interactions, analytic

form factors containing many parameters adjusted to approximate two-body scattering states have been carefully developed.[22–25] The EST formalism has been used here. Scattering states have been approximated at up to four discrete energies. Some of the intended applications are at relativistic energies;[23] nuclear matter calculations have been reported;[24] numerous three-nucleon calculations have been performed.[25] The usefulness of these low rank potentials provides encouragement to attempt to extend separable expansions still further.

The purpose of this paper is twofold. First, we present a computational method for solving the HLS equation at the bound state energy of the potential. For the Malfliet-Tjon (MT) potential V,[26] this energy is -0.35 MeV. In this paper, we only obtain s wave solutions. Our solutions are a finite set of functions $\{\chi_i\}$, called Sturmian functions, that are rational in the variable $x=k^2$.

The second purpose is to apply our method to a known formalism, the UPE, and to investigate convergence through a larger range of energies than previously studied. A separable expansion makes nonhomogeneous Schrödinger or Lippmann-Schwinger integral scattering equations especially simple, reducing them to one-dimensional degenerate kernel equations with algebraic solutions. Furthermore, using our separable potentials, with the $\chi_i(x)$ serving as form factors in the momentum representation, reduces the main work in calculating the k matrix to evaluation of integrals of the form

$$I_{ij}=P\int_{-\infty}^{\infty} dy \frac{y^2\chi_i(y^2)\chi_j(y^2)}{k^2-y^2} .$$

Such integrals are especially easy to perform analytically using residue calculus, since in all cases the $\chi_i(y^2)$ are found to have simple poles on the imaginary axis. As our Padé method produces $\chi_i(y^2)$ in the form of rational functions, analytic residue calculations are in any case possible as long as the $\chi_i(y^2)$ possess no singularities on the real axis and vanish sufficiently rapidly at infinity. We adopt the k-matrix formalism throughout this paper, and all singular integrals are henceforth understood to be Cauchy principal values.

We obtain a new result: at intermediate energies through $E_{\text{c.m.}}=666$ MeV, and at ultrahigh momenta, as the rank of the UPE approaches 13, analytic wave functions (or, equivalently, half-shell k matrices) and phase shifts are found that are in good agreement with precise numerical results. This supplements earlier less complete investigations made at lower energies.[9,18]

We thus address two important issues, analyticity and convergence. That these issues can be treated simultaneously reflects creditably upon our new methods for solving integral equations analytically, which we expect to be applicable to a variety of separable expansion formalisms. The initial choice for this paper, the UPE, was somewhat arbitrary. Other results to be reported later include direct solutions for scattering states.[27] Also, preliminary results show the formalism developed by Harms[28] allows the analytic calculation of Gamow states[29] in momentum space. Hence, we can envision an expanding third category of separable expansions in which the Schrödinger equation or the Lippmann-Schwinger equation is solved to high precision and the resulting momentum space form factors are simple analytic expressions.

Our method is an extension of a recent analytic solution of the s state homogeneous Lippmann-Schwinger (HLS) equation, applied to the UPA,[30] which we refer to in the sequel as I. A restriction has been made to Yukawa-type potentials

$$V(r)=\sum_{j=1}^{N} V_j \frac{\exp(-\mu_j r)}{\mu_j r} . \tag{1.1}$$

Then as shown in I, the s wave HLS equation

$$|\chi_j\rangle=\lambda_j V G_0(E)|\chi_j\rangle , \tag{1.2}$$

where $G_0(E)=[E-(k^2/M)]^{-1}$, is expressible in the form

$$\chi_j(k)=\lambda_j\sum_{p=1}^{N}\frac{g_p}{2\pi}\int_{-\infty}^{\infty} dy\frac{y}{k}\frac{\chi_j(y)}{y^2+\gamma_0^2}\ln[\mu_p^2+(y+k)^2] , \tag{1.3}$$

where natural units are used ($\hbar=c=1$), the strengths are $g_p=-MV_p/\mu_p$ ($M/2$ is the reduced mass), and $\gamma_0^2=MB$ ($B=-E$ is the binding energy). For the Sturmian state with the eigenvalue of smallest modulus, an accurate solution was found,[30] expressed as a rational function of $x=k^2$.

The present work makes use of a redefined inner product; we give a prescription for transforming between two different Hilbert spaces, one a weighted version of the other. This step simplifies the formalism and enables us to find a sequence of N orthonormal Sturmian functions with little change in the computational procedures. In the present application we go to $N=15$. Our Sturmian functions are particularly useful in the UPE, which is simply given by

$$V_N=-\sum_{j=1}^{N}\frac{|\chi_j\rangle\langle\chi_j|}{\lambda_j} , \tag{1.4}$$

with

$$\langle\chi_r|G_0|\chi_s\rangle=-\delta_{rs} . \tag{1.5}$$

The new inner product, defined so as to agree with Eq. (1.5), is used for Gram-Schmidt orthonormalization, which is carried out as an essential part of the construction of the Sturmian functions. Section II presents the formalism, and the Sturmian functions are analyzed in Sec. III.

The issue of convergence of separable expansions was sharpened a long time ago by the observation that a local two-body potential is noncompact in the full two-body Hilbert space,[31] although a separable expansion is necessarily compact. A sequence of compact operators does not produce a convergence approximation to a noncompact operator.[32] Hence no separable expansion can converge in norm to a local potential. It has been pointed out that approximating a local potential by a separable expansion produces the most pronounced discrepancies at high energies, which could be unimportant for low energy nuclear phenomena;[33,34] also, in three-body problems, the relevant operator is not the noncompact $t(z)$, but the compact $t(z)(z-h_0)^{-1}$.[35] Although these early con-

siderations continue to be aired,[36] relativistic applications of separable expansions are also being made.[23] The *in principle* justification of such high energy applications of separable expansions lies in the compactness of the *partial wave* operators $V_l(p,q)$, $t_l(p,q,E)$, and $k_l(p,q,E)$. Several years ago, Chisholm gave a proof that $V_l(p,q)$ and $t_l(p,q,E)$ are compact, for a Yukawa potential.[37] This result is trivially extended to Yukawa-type potentials and to include $k_l(p,q,E)$; also, the proof has recently been extended to include a wider class of local potentials.[27] It therefore follows that for a class of physically meaningful local potentials, separable expansions are not low energy approximations, but instead are finite angular momentum approximations. The noncompactness property only dictates against convergence when the limit $l\to\infty$ is taken.

It is in the light of this insight concerning convergence that we reexamine the UPE for the MT V potential up to a higher energy than before. The earliest UPE calculation for MT V already showed good convergence at $E_{\text{c.m.}}\leq 0$, as needed for trinucleon problems, at rank 3.[9,34] A subsequent investigation[18] of MT V showed 1% errors of phase shifts at $E_{\text{c.m.}}=176$ MeV with a rank 12 UPE (the rank 24 UPE did not do any better). A heuristic analytic basis, when optimized, did significantly better with phase shifts but still showed some 20% discrepancies in the off-shell rank-10 t matrix at $E_{\text{c.m.}}=72$ MeV. Whether these investigations were approaching an energy barrier of convergence peculiar to the UPE has not been resolved. Graz potentials[22] have been carefully fitted to wave functions at several discrete energies up to $E_{\text{lab}}=300$ MeV. This has been done in the EST framework, where special care must be taken to avoid unwanted oscillations, even singularities, at energies not fitted.[13,18,22]

One way to test the fit of an l-wave rank N separable expansion $V_{l,\text{sep}}^N$ to an l-wave local interaction V_l is to calculate a norm error, definable as

$$e(N)=\|V_l-V_{l,\text{sep}}^N\|/[\|V_l\|\,\|V_{l,\text{sep}}^N\|]^{1/2}\ .$$

Compactness of V_l guarantees the existence of a sequence $\{V_{l,\text{sep}}^N\}$ such that $\lim_{N\to\infty}e(N)=0$.[32] We are not aware of NN separable expansions having been tested in this rather exacting way. We conclude there is still some need to better characterize the nature of the practical convergence of separable expansions. In a future paper, we shall address the formal convergence of an SE. Here, we continue to adopt the more informal comparison of phase shifts and k-matrices. Our UPE k matrices give evidence of convergence up to ultrahigh momenta. This is discussed in Sec. IV, where we also illustrate how our solutions can be used with the Ernst-Shakin-Thaler formulation of separable expansions. In the conclusions in Sec. V we also comment further on an extension to Gamow states.

II. FORMALISM

A. Subspace of rational functions

Finding analytic solutions to Eq. (1.3) satisfying the condition Eq. (1.5) is the central problem of this paper. The state of smallest modulus of λ, labeled χ_1, shall be referred to as the HLS ground state. It is found by an iteration procedure that uses Padé approximants.[28] A Padé approximant (PA) is a rational function, here a ratio of two polynomials in the variable x, written $[L/M](x)$ or just $[L/M]$, where L and M are the degrees, respectively, of the numerator polynomial $P_L(x)$ and the denominator polynomial $Q_M(x)$. For normalization, the constant term of $Q_M(x)$ is taken to be just 1. The coefficients of P_L and Q_M may be obtained by solving linear equations that express the equality of the Taylor series of $P_L(x)/Q_m(x)$ and of the function being approximated, through terms of order X^{L+M}.[38]

The solutions $\{\chi_i\}$ are assumed to be rational functions of $x=k^2$ and are found to have poles on the imaginary k axis. To satisfy normalizability of the $\{\chi_i\}$, we have set $M=L+1$. If a rational function $\chi_j(y^2)$ satisfying these conditions is inserted into the right-hand side of Eq. (1.3), the integral is easily evaluated analytically and expanded to obtain a series expansion. More details about this expansion can be found in I. The series is then used to reconstruct the left-hand side of Eq. (1.3) in the same $[L/L+1]$ Padé form, which is then reinserted into the integral on the right-hand side for further iteration. Just a few iterations usually suffice to reach convergence to χ_1 and λ_1. This is similar to the power method for Hermitian matrices.[39]

As with the power method, the task of finding other eigenstates is more complicated. The *ansatz* has been adopted that the Padé denominators, the $Q_M(x)$, can all be the same as found for χ_1. Then if I is the number of poles on the positive imaginary k axis, the PA's are of the type $[I-1/I]$ and form a natural I-dimensional manifold. Orthogonalization is particularly simple because the denominators are identical. If the denominators of two $[I-1/I]$ rational functions are different, a linear combination of them will have a denominator of degree greater than I. Therefore, functions must have the same $Q_I(x)$ denominator to lie in the same I-dimensional space of $[I-1/I]$ functions. An essential step has been to characterize the remaining problem in terms of an Hermitian operator. We now explain how this is done before giving the final details of our procedure.

B. Weighted Hilbert space

Although the potential V is Hermitian, the operator VG_0 is not. As pointed out by Weinberg, Sturmian functions for $E=-B<0$ are simply related to the eigenstates of the Hermitian operator

$$V_h=[-G_0(-B)]^{1/2}V[-G_0(-B)]^{1/2}\ ,$$

and their spectra, the $\{\lambda_j\}$, are identical. Iteration and use of the power method are cumbersome using V_h. It is far simpler to redefine a Hilbert space in which the operator VG_0 is Hermitian.[40] We first note that the operator p^2/M is closed and self-adjoint and $-B$ is in its resolvent set. Consequently,[41] the operator $R=-G_0(-B)$ is bounded and is defined on the entire Hilbert space. Then for all $|\chi\rangle$, R has $(B+p^2/M)$ as its left inverse:

$$(B+p^2/M)R\,|\chi\rangle=|\chi\rangle\ . \tag{2.1}$$

R is also the left inverse of $(B+p^2/M)$ in the domain of definition of p^2/M.

Next, we note that the inner product, defined by

$$\langle\phi\,|\,\psi\rangle'=\langle\phi\,|\,R\,|\,\psi\rangle\ , \tag{2.2}$$

satisfies the axioms for a Hilbert space.[42] In the new space, a weighted version of the old, the matrix element of an operator A is given by

$$\langle\phi\,|\,A\,|\,\psi\rangle'=\langle\phi\,|\,RA\,|\,\psi\rangle\ . \tag{2.3}$$

The usual definition of adjoint applied to the right-hand side gives

$$\langle\psi\,|\,A^{\dagger}R^{\dagger}\,|\,\phi\rangle^*=\langle\psi\,|\,RR^{-1}A^{\dagger}R\,|\,\phi\rangle^*=\langle\phi\,|\,RA\,|\,\psi\rangle\ . \tag{2.4}$$

It follows that the adjoint of A, written $\overline{A}$ in the new space, is given by

$$\overline{A}=R^{-1}A^{\dagger}R\ . \tag{2.5}$$

In the new space, we find $\overline{V}\overline{R}=R^{-1}RVR=VR$ and hence VR is Hermitian. Henceforth, we shall work entirely in the new space, writing $\langle\phi\,|\,\psi\rangle$ for $\langle\phi\,|\,\psi\rangle'$ and $A^{\dagger}$ for $\overline{A}$. The orthogonality condition of Eq. (1.5) is now simply expressed as

$$\langle\chi_i\,|\,\chi_j\rangle=\delta_{ij}\ . \tag{2.6}$$

This completes the formulation of the eigenvalue problem in terms of a Hermitian operator. We may now easily take advantage of the simple structure of our $[I-1/I]$ manifold. We first construct the $I-1$ dimensional subspace orthogonal to the first Sturmian state by Gram-Schmidt orthonormalization. Finally, we use the inverse power method,[39] which we have found to be a fast and accurate way to determine the remaining eigenfunctions and spectrum.

III. STURMIAN FUNCTIONS

A. Spectrum for Malfliet-Tjon potential V

We present results for the Malfliet-Tjon potential V (MT V), a spin-averaged np interaction with a two-body bound state at $E=-0.35$ MeV.[18] The parametrization is

$$V=V_1\frac{\exp(-\mu_1 r)}{\mu_1 r}+V_2\frac{\exp(-\mu_2 r)}{\mu_2 r}\ , \tag{3.1}$$

where, in natural units,

$$V_1=-4.4800608\ \text{fm}^{-1},\quad V_2=22.671974\ \text{fm}^{-1}\ ,$$

$$\mu_1=1.55\ \text{fm}^{-1},\quad \mu_2=3.11\ \text{fm}^{-1}\ ,$$

with the physical constants[25]

$$(\hbar c)^{-1}=5.0676896\times10^{-3}\ \text{fm}^{-1}/\text{MeV}=1$$

and

$$(M)^{-1}=0.21016417\ \text{fm}\ .$$

Calculations have been performed on the URI IBM 4381-3 mainframe, almost entirely in extended precision (32 figures). We have sometimes found such high precision to be necessary for accurately determining roots of polynomials of our denominator of degree 15 or greater. Excellent values of these roots are needed in the residue calculations for analytic evaluation and series expansion of Eq. (1.3). When double precision is used, the poles of the $\chi_i(y^2)$ sometimes even erroneously appear off the imaginary k axis. This occurs because polynomial root finding is an intrinsically ill-conditioned problem which loses much precision, even though the algorithm we use, the Bairstow method, is easily programmed.[43] The rest of our results are fairly stable when 16-figure precision is used. Although the MT V potential lacks a tensor term, it provides a better example than a more physically realistic central singlet np potential because it has a bound state and an earlier numerical study of its Lippmann-Schwinger spectrum is available.[28] We have determined the s-wave scattering function, $F(k^2)=k\cot(\delta_0)$; as shown in Fig. 1, there is a pole near $k=2$ fm^{-1} where the phase shift is zero. Figure 1, when compared with Fig. 3 of Ref. 44, indicates a weaker short-range repulsion than that of the Reid soft core potential. The behavior of the phase shifts at $k\approx100$ fm^{-1}, far beyond the range of validity of our nonrelativistic theory, is only relevant to nuclear physics insofar as it is a measure of the strength of the saturating effect of the short-range repulsion.

Table I gives our computed spectrum through the first nine eigenvalues. We see that as the dimension of the subspace of Sturmian functions increases, the spectrum approaches Harms's results. For a check, we have been able to reproduce Harms's results to within one percent by first converting the HLS equation to a system of linear equations using 64 point Gaussian quadrature and then applying standard methods for solving the eigenvalue problem for a general nonsymmetric matrix.[42] Figure 2 shows our first two attractive eigenfunctions (i.e., for $\lambda_j>0$); Fig. 3 shows the first repulsive eigenfunctions. They are in good agreement with the tabulated values of

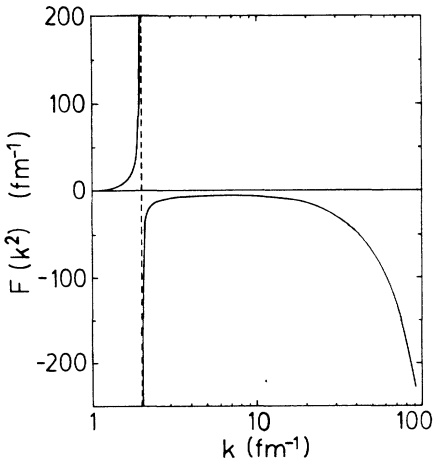

FIG. 1. Scattering function, $F(k^2)=k\cot(\delta_0)$, for MT V potential. Pole is at $k=1.991$ fm^{-1}.

TABLE I. PA spectrum of Lippmann-Schwinger kernel for Malfliet-Tjon potential V (Ref. 26), which appears to converge as I, the number of poles of χ_j on the positive imaginary axis, increases from 8 to 15. The last column gives the result of Harms's numerical calculation, which we have independently verified. All of Harms's λ's are shown. Our [7/8] case did not have a fourth repulsive eigenvalue, λ_6.

	Padé Approximant			
Eigenvalue	[7/8]	[11/12]	[14/15]	Harms
λ_1	−0.433 889	−0.434 077	−0.434 053	−0.4342
λ_2	0.999 999	0.999 995	0.999 995	1.000
λ_3	−1.784 70	−1.777 60	−1.776 81	−1.777
λ_4	−5.397 74	−4.230 89	−4.020 69	−3.881
λ_5	7.269 52	7.219 97	7.218 44	7.218
λ_6		−15.4122	−9.527 03	
λ_7	22.4815	19.5634	19.3133	19.27
λ_8	73.8954	41.2485	38.0491	36.66
λ_9	484.393	89.4164	73.4903	

Harms. In Fig. 3, the third repulsive eigenfunction has been smoothed to remove small oscillations at $k \leq 1$ fm^{-1}. These oscillations appear to be artifacts of our 64-point Gauss-Legendre (GL) quadratures, used in this paper throughout for calculating matrix elements and solving integral equations.[45] We have converted momentum space integrals in the range 0 to ∞ to integrals in y in the range -1 to $+1$ by the transformation[46]

$$k = c\frac{1-y}{1+y}$$

and we have found $c = 10$ to be optimum. When we have used 200 point GL quadrature, and also when we have let I increase to near 20, these oscillations are diminished, but not eliminated.

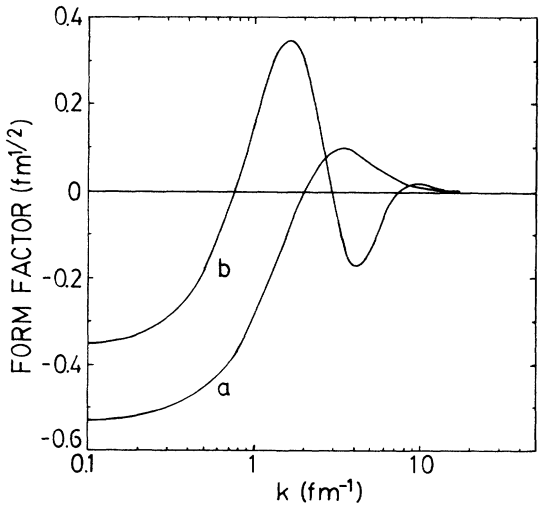

FIG. 2. First two attractive eigenfunctions of the HLS equation for MT V potential. Curve a is associated with $\lambda_1 = 1.000$ and the bound states; it has a node at $k = 1.982$ fm^{-1}.

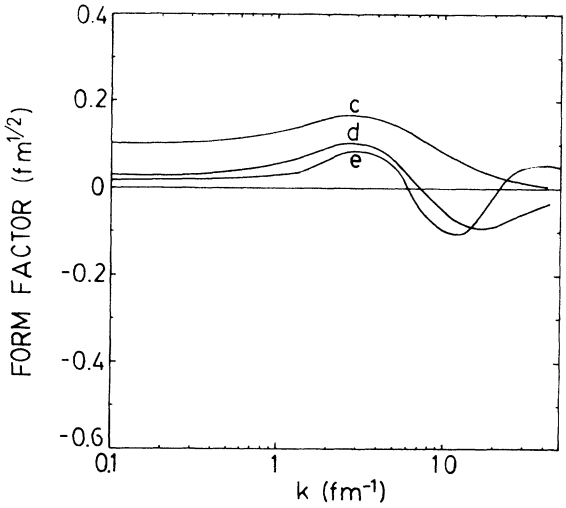

FIG. 3. First three repulsive eigenfunctions of the HLS equation for MT V potential. Curves c, d, and e are in order of increasing magnitude of λ.

B. Reconstructed potentials

If a bound state is known exactly and analytically, a local potential which produces that state can be constructed. In the present context, this amount to a reconstruction of the original local potential. An exacting check can therefore be made of the accuracy of the wave function. The potential is computed from the Schrödinger equation:

$$\bar{V}(r) = \frac{u''(r) - \gamma_0^2 u(r)}{u(r)} , \tag{3.2}$$

where the solution $\psi(r) = u(r)/r$ is obtained by Fourier-transforming the second HLS state $\psi(k) = \chi_2(k)/(k^2+\gamma_0^2)$ to give

$$\psi(r) = \frac{1}{r}\sum_{j=1}^{I} \frac{c_j}{q_j^2 - \gamma_0^2}(e^{-\gamma_0 r} - e^{-q_j r}) . \tag{3.3}$$

The poles of $\chi_2(k)$ are given by $\{\pm iq_j\}$. The reconstructed potential takes the form

$$\bar{V}(r) = -\frac{\sum_{j=1}^{I} c_j e^{-q_j r}}{\sum_{j=1}^{I} \frac{c_j}{q_j^2 - \gamma_0^2}(e^{-\gamma_0 r} - e^{-q_j r})} . \tag{3.4}$$

The potential $\bar{V}(r)$ has been reconstructed from the [7/8], the [11/12], and the [14/15] wave functions. In Table II numerical values are given for these three potentials together with the exact potential.

Except for small and unimportant oscillations in the extreme end of the tail (starting at 10.8 fm for the [14/15] case), a high precision convergence is seen as I increases. The extreme short-range asymptotic form is $\bar{V}(r) \sim a_I / r$, where the exact a is 4.40, $a_8 = 5.98$, $a_{12} = 4.33 = a_{15}$.

Finally, the reconstructed potentials have been used to

TABLE II. Reconstructed MT V potential. The bound state $\psi(p)=\chi_2(p)/(p^2+\gamma_0^2)$ has been Fourier transformed and then used in Eq. (3.4) to produce $\bar{V}(r)$. Convergence with increasing I in $[I-1/I]$ is seen at all radial distances r. (The entry 0.278 58[+2] reads 0.27858×10^2.)

r (fm)	[7/8] (fm^{-1})	[11/12] (fm^{-1})	[14/15] (fm^{-1})	Exact (fm^{-1})
0.1	0.278 58[+2]	0.287 00[+2]	0.286 98[+2]	0.286 62[+2]
0.3	0.354 99[+1]	0.350 66[+1]	0.350 66[+1]	0.350 72[+1]
0.5	0.405 75[0]	0.416 01[0]	0.416 00[0]	0.415 95[0]
1.0	−0.286 25[0]	−0.288 32[0]	−0.288 32[0]	−0.288 33[0]
2.0	−0.577 29[−1]	−0.578 53[−1]	−0.578 55[−1]	−0.578 53[−1]
3.0	−0.898 51[−2]	−0.899 47[−2]	−0.899 58[−2]	−0.899 66[−2]
4.0	−0.166 28[−2]	−0.146 04[−2]	−0.145 93[−2]	−0.145 92[−2]
5.0	−0.226 55[−3]	−0.248 07[−3]	−0.248 67[−3]	−0.248 74[−3]
6.0	−0.333 87[−4]	−0.438 92[−4]	−0.442 65[−4]	−0.440 32[−4]
8.0	−0.188 25[−4]	−0.167 63[−5]	−0.147 04[−5]	−0.148 80[−5]

calculate s wave phase shifts, and as seen in Table III, the excellent agreement shown there is a final convincing demonstration of the accuracy of the ground state wave function.

IV. SEPARABLE EXPANSIONS

A. Unitary pole approximation (UPA)

It is convenient to renumber the HLS eigenfunctions so that the first, $\chi_1(k)$, will be associated with the eigenvalue 1 and the first term in the expansion of Eq. (1.4). The UPA is then the rank 1 s-wave potential

$$V_1=-|\chi_1\rangle\langle\chi_1| \ . \tag{4.1}$$

Solving for the s-wave k matrix (k_0) gives the s-wave scattering function $F_1(k^2)=k\cot(\delta_0)$ as

$$F_1(k^2)=-\frac{2}{\pi M}k_0^{-1}=\frac{2}{\pi M}\frac{1+J(k^2)}{\chi^2(k^2)} \ , \tag{4.2}$$

where the Cauchy principal value integral $J(k^2)$ is

$$J(k^2)=M\int_0^\infty dy\frac{y^2\chi^2(y^2)}{k^2-y^2} \ . \tag{4.3}$$

TABLE III. S-wave phase shifts for the potentials defined in Table II.

k (fm^{-1})	[7/8] (deg)	[11/12] (deg)	[14/15] (deg)	Exact (deg)
0.1	−54.737	−54.767	−54.767	−54.767
0.3	83.492	85.516	85.517	85.517
0.5	65.924	66.003	66.003	66.003
1.0	35.135	35.088	35.088	35.088
1.3	22.057	22.057	22.057	22.057
1.5	14.699	14.738	14.738	14.738
2.0	−27.313	−23.518	−23.514	−23.553
3.0	−21.116	−21.163	−21.163	−21.163
10.0	−61.181	−61.236	−61.235	−61.239
20.0	−56.069	−56.400	−56.397	−56.348

The scattering length and effective range are simply

$$a=-F(0)^{-1}, \quad r_0=2\frac{dF(0)}{dk^2} \ . \tag{4.4}$$

These functions are easily evaluated in terms of the Padé coefficients. The effective range parameters of V_1 are given in the next section. These are in excellent agreement with the effective range parameters calculated using the Malfliet-Tjon potential V and the method of Ref. 47. Other approximations shown in the tables are discussed in the next two sections.

The node of χ_1 at $k_n=1.9822$ fm^{-1} produces a double pole in $F(k^2)$ and a double zero in the phase shift remarkably close to the exact zero of the phase shift associated with V at $k=1.9901$ fm^{-1}. Although the phase shift from V_1 does not change sign at this value of k, the form factor $\chi_1(k^2)$ clearly contains some effects of the repulsion in the MT V potential. As seen in Table IV, the node of χ_1 pulls the phase shifts for V_1 into qualitative agreement with the phase shift for V up to $k\simeq2$ fm^{-1}.

B. Unitary pole expansion (UPE)

We consider a rank-2 approximant with $|\chi_1\rangle$ and $|\chi_2\rangle$, which we call V_2; a rank-3 approximant with $|\chi_1\rangle$ and $|\chi_2\rangle$ and the next attractive form factor $|\chi_5\rangle$, labeled V_3;[9] and higher rank-n approximants, V_n, which use the first n terms. Scattering state wave functions and effective range parameters are expressible in terms of the scattering functions

$$F_i=\frac{2}{\pi M}\frac{\lambda_i+J_{ii}(k^2)}{\chi_i^2(k^2)} \ , \tag{4.5}$$

where

$$J_{ij}(k^2)=M\int_0^\infty dy\frac{y^2\chi_i(y^2)\chi_j(y^2)}{k^2-y^2} \tag{4.6}$$

and

TABLE IV. S-wave phase shifts for the MT V potential and various approximants. The rank-2 EST potential was constructed so as to give the rank-15 wave function at $k=2.9$ fm^{-1}. The rank-15 and rank-13 phase shifts are equal to four significant figures in the momentum range shown.

k (fm^{-1})	V exact (deg)	V_1 (deg)	V_2 (deg)	V_2 EST (deg)	V_{13} (deg)
0.1	−54.77	−54.79	−54.79	−54.80	−54.78
0.5	66.00	64.55	64.45	64.41	65.96
1.0	35.09	29.15	28.29	28.05	35.06
1.9	2.45	0.21	−9.36	−8.28	2.32
2.0	−0.24	0.01	−11.69	−10.08	−0.42
2.5	−11.86	5.99	−19.10	−14.97	−12.01
3.0	−21.16	13.39	−22.41	−21.30	−21.13
4.0	−34.95	13.67	−28.44	−54.34	−35.10
5.0	−44.36	8.37	−36.37	−90.05	−44.99
6.0	−50.83	4.47	−43.61	−116.08	−52.92

$$R_{ij}=\frac{J_{ij}(k^2)}{\pi\chi_i(k^2)\chi_j(k^2)} \ . \tag{4.7}$$

For the rank-2 potential V_2, the scattering function is

$$F=\frac{F_1F_2-R_{12}}{F_1+F_2-2R_{12}} \ , \tag{4.8}$$

while the scattering length and effective range are[48]

$$a=\frac{a_1+a_2+2a_1a_2R_{12}(0)}{1-a_1a_2R_{12}^2(0)} \tag{4.9}$$

and

$$r=\left[a_1r_1+a_2r_2+4a_1a_2R_{12}(0)\frac{dR_{12}(0)}{dk^2}\right]\Big/Q$$
$$-a_1a_2[1-a_1a_2R_{12}^2(0)]\left[r_1+r_2-4\frac{dR_{12}(0)}{dk^2}\right]\Big/Q^2 \ , \tag{4.10}$$

where $Q=a_1+a_2+2a_1a_2R_{12}(0)$. The rank 2 effective range parameters (a_1,r_1) and (a_2,r_2) are associated with the form factors $|\chi_1\rangle$ and $|\chi_2\rangle$, respectively. Our exact values are $a=12.1702$ fm and $r=2.30288$ fm, compared with our UPA values of $a=12.1726$ fm and $r=2.30990$ fm. In accordance with expectations, our higher rank values show very little variability: $\approx 0.01\%$ for a and $\approx 0.1\%$ for r.

The Schrödinger equation for the s-wave scattering state is

$$\psi_{0k}(p)=\frac{\delta(p-k)}{p^2}+\frac{M}{k^2-p^2}W(k,p) \ , \tag{4.11}$$

where $W(k,p)$ is the half-shell k matrix. Wave function convergence, which is half-shell k-matrix convergence, is a more stringent test of separable expansions than phase shift convergence. We study both.

For V_n, the k matrix is obtained by algebraic means, the details of which we do not give. The precise numerical solution for the original potential follows a standard procedure[49] using 64-point Gauss-Legendre quadrature. Table IV shows convergence of phase shifts through 6.0 fm^{-1}, and Figs. 4 through 7 reveal half-shell k-matrix convergence at CM energies as high as 666 MeV (4.0 fm^{-1}) for wave numbers as high as 12 fm^{-1}. The Noyes-Kowalski half-shell function[50]

$$f(p,q)=\frac{k_0(p,q,E)}{k_0(q,q,E)}, \quad q^2/M=E \tag{4.12}$$

has been shown here. A completely off-shell k matrix is also shown in Fig. 8. For fixed k, the rank-n half-shell k matrix has the form

$$W(q,p)=\sum_{j=1}^{n} b_j(q)\chi_j(p) \ . \tag{4.13}$$

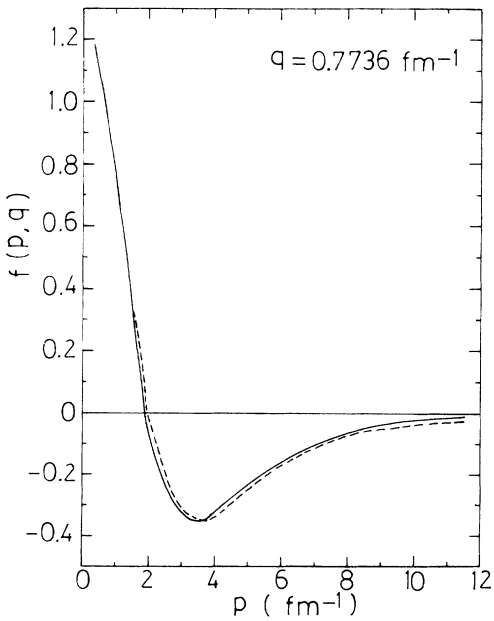

FIG. 4. S-wave Noyes-Kowalski function for MT V potential at $E_{\text{c.m.}}=24.9$ MeV. The solid curve is exact and coincides with our rank-13 result. — — — is our rank-3 UPE result.

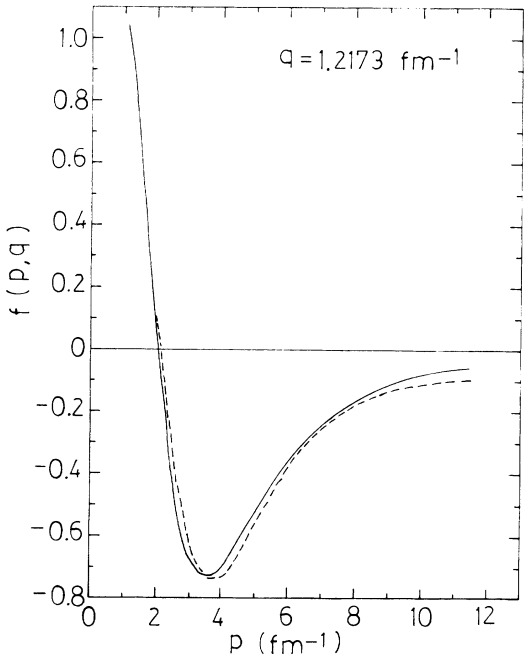

FIG. 5. Same as Fig. 4 at $E_{\text{c.m}} = 61.7$ MeV.

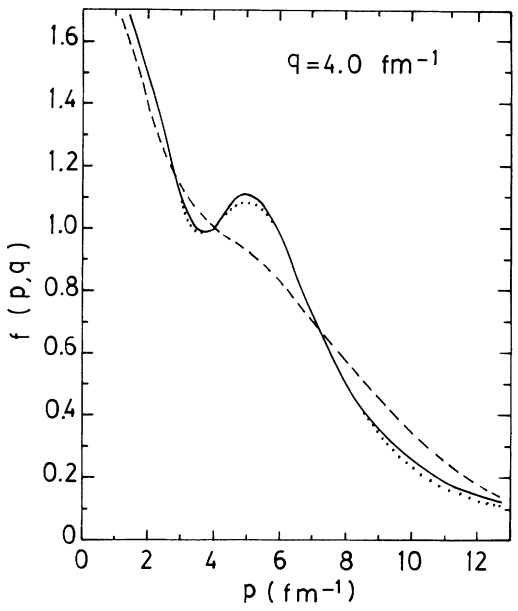

FIG. 7. Same as Fig. 6 at $E_{\text{c.m.}} = 666$ MeV.

This is a simple yet accurate rational approximant to the wave function. Statistical Padé approximant methods[47,51] would have enabled us to find analytic forms for the $b_j(q)$, too, had we wished to.

Our rank-15 calculations show convergence and hence constitute a constructive proof of the ability of a particular separable expansion to approximate a local potential in the s wave. Nonetheless, the value of a separable expansion diminishes as the required rank grows. We conclude this section with an illustrative application of the EST method which attempts to optimize a rank-2 expansion. This is done by treating the rank-15 problem as exact, while identifying the rank-2 form factors $|\phi_1\rangle$

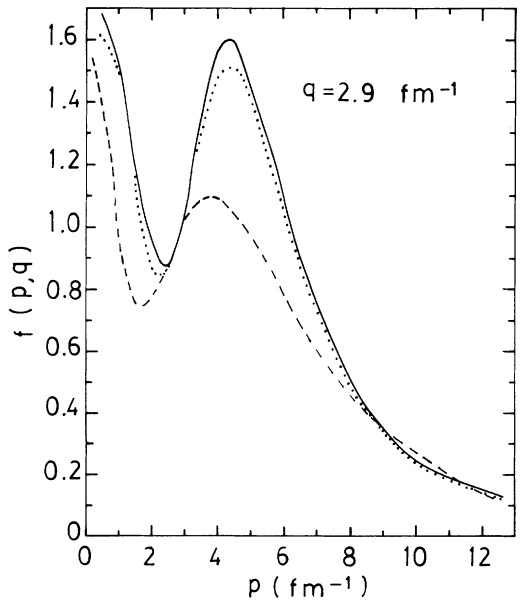

FIG. 6. S-wave Noyes-Kowalski function for MT V potential at $E_{\text{c.m.}} = 350$ MeV. The solid curve is exact and coincides with our rank-13 result and our rank-2 EST result; · · · · is our rank-8 result; — — — is our rank-5 result.

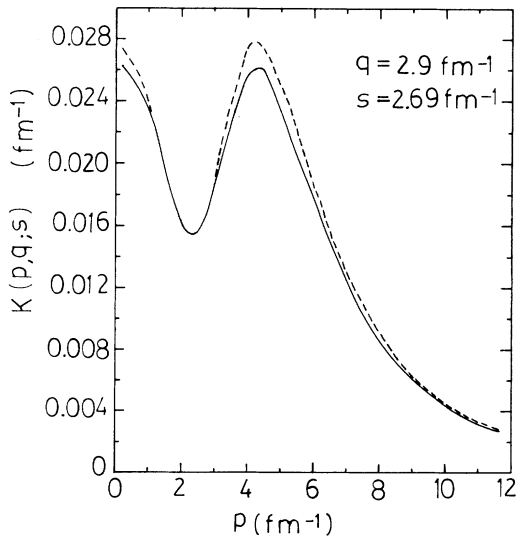

FIG. 8. S-wave completely off-shell k matrix for MT V potential at $E_{\text{c.m.}} = 350$ MeV. The solid curve is exact and coincides with our rank-13 result. — — — is our rank-2 EST result.

and $|\phi_2\rangle$ as $|\phi_1\rangle = |\chi_1\rangle$ and $|\phi_2\rangle = \sum_{j=2}^{15} a_{2j} |\chi_j\rangle$. The a_{2j} are determined by solving the rank-2 and rank-15 problems and equating the two half-shell k matrices at wave number q. The resulting equations for the a_{2j} are only consistent in a limited range of energy. Even where they are consistent, we sometimes obtain two attractive form factors. The lowest q at which a solution exists that produces one repulsive and one attractive form factor is $q = 2.9$ fm^{-1}. At this q, the rank-2 and rank-15 analytical wave functions are identical. This means the half-shell rank-2 k matrix is exact at this energy. As seen in Table IV, this potential gives phase shifts comparable to or slightly better than those of the UPE rank-2 potential, up through 3 fm^{-1}, but is significantly over-repulsive at higher wave numbers. This is because the strength of the rank-2 repulsive term has become unrealistically large. Here we primarily wish to draw attention to the ease with which the available analytic expressions can be manipulated, simplifying heuristic EST calculations.

V. CONCLUSIONS

A new method for solving integral equations has been developed and applied to the homogeneous Lippmann-Schwinger equation in momentum space. The new feature is that solutions are analytic expressions, obtained as Padé approximants in the variable $x = k^2$. As developed here, the method is applicable whenever the energy assumed is less than or equal to zero. In conjunction with the formulation of Harms,[28] this method has been extended to antibound states, which will be discussed in a future paper.[29] We have presented results for the Malfliet-Tjon V potential, where the assumed energy, $E = -0.35$ MeV, is the physical two-body bound state energy associated with this potential. A finite subspace of rational functions with fixed denominators has been constructed, wherein Sturmian eigenfunctions and eigenvalues show convergence even for rather low ($N \leq 15$) dimensions. Applications have so far been restricted to Yukawa-type potentials in order for Eq. (1.3) to be expanded as a series analytically and summed using Padé approximants. Future applications can be made with a larger class of potentials, because if a strictly numerical evaluation of the integrals is performed, some statistical Padé techniques can achieve comparable results.[47,51]

As a further application and test of the method, a separable expansion of the Malfliet-Tjon potential V, the unitary pole expansion, has been directly constructed from the Stumian eigenstates. As the rank N approaches 15, convergence is seen of phase shifts, the half-shell k matrix, and the completely off-shell k matrix up through $E_{\text{c.m.}} = 666$ MeV. Such high-energy convergence to accurate values associated with the original local potential is a new result. There is a straightforward explanation. All partial wave projections of Yukawa-type central potentials are compact, and can therefore be arbitrarily well approximated by operators of finite rank. Hence separable expansions need not in principle be reserved for low-energy use. Still, two-body local potentials are not compact in the full two-particle Hilbert space. This noncompactness is associated with the limit $l = \infty$; consequently, separable expansions should be applicable to any problem as long as only a finite number of partial waves is involved.

The convergence rate of the UPE we obtain is probably too slow for high-precision calculations of nuclear structure and nuclear reactions when several partial waves contribute. Alternative separable expansion formalisms can also utilize the method we present for constructing analytic form factors that are solutions of a dynamical problem. As an illustration, we have carried out an EST calculation to generate a rank-2 potential that gives exactly the same wave functions for $q = 2.9$ fm^{-1} as the excellent rank-15 approximant. Gamow states appear to lead to a rapidly converging separable expansion.[13] They are currently under investigation. A recent rational S-matrix method[47] locates the bound state and antibound state poles and the Gamow states nearest the origin, and appears to be a useful tool in solving the Gamow state eigenvalue problem. It is also our intention to extend the present investigations to problems having coupled partial waves.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge valuable discussions with J. Bonner, L. Kahn, C. Kaufman, R. Kidwell, and P. Nightingale. We are particularly indebted to L. Kahn for his careful reading of the manuscript. The URI academic computer center has generously provided time on the URI IBM 4381-3 mainframe.

[1] M. Lacombe *et al.*, Phys. Rev. C **21**, 861 (1980).
[2] R. Machleidt and K. Holinde, in *Few Body Problems in Physics*, edited by B. Zeitnitz (Elsevier, Amsterdam, 1984), Vol. II, p. 57.
[3] G. Brown and A. Jackson, *The Nucleon-Nucleon Interaction* (North-Holland/American Elsevier, New York, 1976).
[4] Y. Yamaguchi, Phys. Rev. **95**, 1628 (1954); Y. Yamaguchi and Y. Yamaguchi, Phys. Rev. **95**, 1635 (1954).
[5] A. Mitra, Nucl. Phys. **32**, 529 (1962); A. Mitra, in *Advances in Nuclear Physics*, edited by M. Baranger and E. Vogt (Plenum, New York, 1969).
[6] S. Adhikari and L. Tomio, Phys. Rev. C **33**, 467 (1985).
[7] S. Weinberg, Phys. Rev. **131**, 440 (1963).
[8] M. Fuda, Nucl. Phys. **A116**, 83 (1968).
[9] E. Harms, Phys. Rev. C **1**, 1667 (1970); B. Siebert, J. S. Levinger, and E. Harms, Nucl. Phys. **A197**, 33 (1972).
[10] G. Rawitscher, Phys. Rev. C **25**, 2196 (1982); G. Rawitscher and G. Delic, *ibid.* **29**, 1153 (1984).
[11] D. Ernst, C. Shakin, and R. Thaler, Phys. Rev. C **8**, 46 (1973); D. Ernst, C. Shakin, R. Thaler, and D. Weiss, *ibid.* **8**, 2056 (1973).
[12] B. Gyarmati and A. Kruppa, Phys. Rev. C **34**, 95 (1986); B. Gyarmati, A. Kruppa, Z. Papp, and A. Wolf, Nucl. Phys. **A417**, 393 (1984); B. Gyarmati and A. Kruppa, *ibid.* **A378**, 407 (1982); B. Gyarmati, A. Kruppa, and J. Révai, Nucl. Phys. **A326**, 119 (1979).

[13]M. Baldo, L. Ferreira, L. Streit, and T. Vertse, Phys. Rev. C **33**, 1587 (1986); M. Baldo, L. Ferreira, and L. Streit, *ibid.* **32**, 685 (1985); R. C. Fuller, Phys. Rev. **118**, 1649 (1969).
[14]S. Oryu, Phys. Rev. C **27**, 2500 (1983).
[15]S. Oryu, Prog. Theor. Phys. **62**, 847 (1979); S. Oryu, M. Araki, and S. Satoh, Prog. Theor. Phys. Suppl. **61**, 199 (1977); S. Oryu, *ibid.* **61**, 180 (1977); S. Oryu, Prog. Theor. Phys. **52**, 550 (1974).
[16]C. Baker, *The Numerical Treatment of Integral Equations* (Clarendon, Oxford, 1977).
[17]J. Horáček and T. Sasakawa, Phys. Rev. C **32**, 70 (1985); Phys. Rev. A **30**, 2274 (1984); **28**, 2151 (1983).
[18]S. Adhikari and I. Sloan, Phys. Rev. C **11**, 1133 (1975).
[19]S. Adhikari and I. Sloan, Nucl. Phys. **A241**, 429 (1975).
[20]S. Adhikari, Phys. Rev. C **10**, 1623 (1974).
[21]W. Glöckle, *The Quantum Mechanical Few-Body Problem* (Springer, Berlin, 1983).
[22]J. Haidenbauer, Y. Koike, and W. Plessas, Phys. Rev. C **33**, 439 (1986); J. Haidenbauer and W. Plessas, *ibid.* **32**, 1424 (1985); W. Schweiger, J. Haidenbauer, and W. Plessas, *ibid.* **32**, 1261 (1985); J. Haidenbauer and W. Plessas, *ibid.* **30**, 1822 (1984); **27**, 63 (1983); L. Matelitsch, W. Plessas, and W. Schweiger, *ibid.* **26**, 65 (1982).
[23]K. Schwarz, J. Haidenbauer, and J. Frohlich, Phys. Rev. C **33**, 456 (1986); L. Matelitsch and H. Garcilazo, *ibid.* **32**, 1635 (1985).
[24]H. Lampl and M. Weigel, Phys. Rev. C **33**, 1834 (1986).
[25]Y. Koike, J. Haidenbauer, and W. Plessas, Phys. Rev. C **35**, 396 (1987); B. Loiseau, L. Matelitsch, W. Plessas, and K. Schwarz, *ibid.* **32**, 2165 (1965); Y. Koike, W. Plessas, and H. Zankel, *ibid.* **32**, 1796 (1985); H. Zankel and W. Plessas, Z. Phys. A **317**, 45 (1984); H. Zankel, W. Plessas, and J. Haidenbauer, Phys. Rev. C **28**, 538 (1983).
[26]R. Malfliet and J. Tjon, Nucl. Phys. **A127**, 161 (1969).
[27]K. Hartt (unpublished).
[28]E. Harms, Ph.D. thesis, Rensselaer Polytechnic Institute, 1969 (unpublished).
[29]V. Yidana and K. Hartt (unpublished).
[30]K. Hartt, Phys. Rev. C **26**, 2616 (1982).
[31]T. Osborn, J. Math. Phys. **14**, 373 (1973).
[32]R. Newton, *Scattering Theory of Waves and Particles*, 2nd ed. (Springer, New York, 1982).
[33]J. Levinger, J. Math. Phys. **14**, 1314 (1973).
[34]J. Levinger, in *Nuclear Physics*, Vol. 71 of *Springer Tracts in Modern Physics*, edited by G. Hohler (Springer, Berlin, 1974).
[35]I. Sloan and J. Gray, Phys. Lett. **44B**, 354 (1973).
[36]J. Haidenbauer and Y. Koike, Phys. Rev. C **34**, 1187 (1986).
[37]J. Chisholm, in *The Padé Approximant in Theoretical Physics*, edited by G. Baker, Jr. and J. Gammel (Academic, New York, 1970), p. 171.
[38]G. Baker, Jr., *Essentials of Padé Approximants* (Academic, New York, 1975).
[39]L. Johnson and R. Riess, *Numerical Analysis*, 2nd ed. (Addison-Wesley, Reading, 1982).
[40]C. Cohen-Tannoudji, B. Diu, and F. Laloe, *Quantum Mechanics* (Herman, Paris, 1977), Vols. 1 and 2.
[41]N. Dunford and J. Schwartz, *Linear Operators, Part I: General Theory* (Interscience, New York, 1957).
[42]G. Dahlquist and A. Björck, *Numerical Methods* (Prentice-Hall, Englewood Cliffs, New Jersey, 1974).
[43]M. Maron, *Numerical Analysis* (Macmillan, New York, 1982).
[44]K. Hartt, Phys. Rev. C **23**, 2399 (1981).
[45]C. Love, *Abscissas and Weights for Gaussian Quadrature* (National Bureau of Standards Monograph 98, U. S. Government Printing Office, Washington, D. C., 1966).
[46]L. Tomio and S. Adhikari, Phys. Rev. C **24**, 43 (1981).
[47]K. Hartt and P. Yidana, Phys. Rev. C **31**, 1105 (1985).
[48]This corrects the sign error in the rank 2 scattering length given in Ref. 30.
[49]G. Brown, A. Jackson, and T. Kuo, Nucl. Phys. **A133**, 481 (1969).
[50]H. Noyes, Phys. Rev. Lett. **15**, 538 (1965).
[51]V. Krasnopolsky, V. Kukulin, and J. Horáček, Czech. J. Phys. B **35**, 818 (1985).