The Formation of a Rational S Matrix Using Phase Shifts from Elastic Scattering

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Three linear methods for constructing a rational S matrix from phase shifts are presented and compared. Applications to $^1S_0$ neutron–proton elastic scattering data and to potential model problems show them to be efficient and in some cases superior to the Newton–Raphson (NR) and Levenberg–Marquardt (LM) methods. The relative power of the three methods is seen to depend upon the smoothness of the data. One exacting test we have made is to take as data some phase shifts computed to high accuracy from a spin-averaged NN potential of Malfliet and Tjon (MTV). We truncate the MTV potential at different ranges R. The known analytic structure resulting from the truncation, including Gamow state poles, is stably reproduced. One method, which we designate as KKH, is superior in this problem with smooth data. In another class of problems, when even small random noise is injected into our neutron–proton data, another method, which we label HY, is superior. In this case, LM, NR, and KKH are sometimes completely ineffective. Slight improvements are sometimes made with NR or LM iterations after the other methods have achieved their optimum parameter values. Therefore, we recommend that all five methods be programmed together as different options. Such a program should contain a number of important rational function checks. © 1988 Academic Press, Inc.

1. INTRODUCTION

The S matrix is a fundamental construct in scattering theory. In this paper we present and compare stratagems for the formation of an approximate S matrix that contains a rational function of momentum, from experimentally or theoretically derived elastic phase shifts. The need for such stratagems becomes clear in the context of current scattering theory as applied to nuclear physics. For a given angular momentum, bound states, antibound states, and resonances appear in the S matrix as simple poles [1]. In one case of practical interest, which we shall refer to as case (a), the S matrix is approximated as a rational function of k. Such an approximation has been successfully used to construct NN potentials [2–5]. Inverse scattering theory is easily applied in case (a) to produce separable [5, 6] or local [2–4] potentials. In another case which we call case (b), the S matrix is expressed as $S(k) = \exp[-2ikR] D(k)$, where $D(k)$ is a function in k with an infinite number of poles and zeros. For a local potential which is of compact support, the latter case is known to be a more accurate representation of the S matrix and R is then the range beyond which the potential vanishes [7]. The ability to

481

approximate $S(k)$ or $\exp[2ikR]\, S(k)$ as a rational function of the momentum k in the center of the momentum system, characterized entirely in terms of zeros and poles, is therefore useful.

In nuclear physics, recent work has shown that nucleon–nucleon (NN) interactions representable as sums of Yukawas are well approximated by rational S matrices [8] and that a variety of nuclear systems can be effectively represented in this way [9]. Poles of the S matrix can be computed accurately from precisely known phase shift data [8]. Recently, Gamow state poles have been accurately located in this way [10] for the Reid soft core (RSC) NN $^1S_0$ potential [11]. Locating those poles is a useful step in the application of one of the more powerful separable expansion techniques developed recently [12, 13]. Finally, a current nuclear physics problem, the unequivocal identification of a dibaryon resonance in medium energy NN scattering [14], would be simplified if the S matrix for the relevant states were well approximated by a rational function. All the problems we have mentioned can be reduced to a minimization of χ^2.

Here, we investigate three newer alternative methods for minimizing χ^2. We compare them with two standard methods, Newton–Raphson (NR) [15, 16] and Levenberg–Marquardt (LM) [16–18]. The NR method requires a tedious evaluation of the derivative matrix $M_{ij} = \partial^2\chi^2/\partial\alpha_i\partial\alpha_j$ at each iteration point. This makes NR relatively slow, but it continues to be a method of choice in some problems such as calculations of polynomial roots when the derivatives are simple to evaluate, because of good convergence properties [15]. Since LM is especially tailored to minimizing a sum of squares and only requires knowledge of the Jacobian matrix of χ^2, the LM iterations are fast. Here we use an even faster version of LM that approximates derivatives using finite differences [16, 18]. However, it is found that the convergence rate per step of LM is slow, and that both LM and NR frequently do not converge at all. Newton method variants are of continuing importance in computational physics [19, 20]; in this case, comparisons with the Newton–Raphson method provide important benchmarks.

Typically, the analysis of elastic scattering data results in numerical tables of phase shifts for real non-negative k. The partial wave S matrix for a central interaction, $S_l(k) = \exp[2i\delta_l(k)]$, can be continued to the complex k plane by the ansatz (a) that it be rational or (b) that it have a structure $\exp[-2ikR]\, D(k)$, where $D(k)$ is rational. For case (a), transforming phase shifts into values of the scattering function $F_l(k) = k^{2l+1}\cot[\delta_l(k)]$ is a convenient procedure. Unlike the phase shift $\delta_l(k)$, the function $F_l(k)$ has a structure of poles and zeros that makes it ideally representable as rational function. The function $F_l(k)$ is even [1]. Hence, the technical problem can be posed in terms of the variable $x = k^2$: find a meromorphic continuation of a discrete function $F_l(x_j)$, where $j = 1, 2, ..., N$.

Hereafter, we shall restrict our analysis to the s wave. Then case (b) is characterized by the equation

$$D(k) = \frac{G(k^2) + ik}{G(k^2) - ik},\qquad (1)$$

since G is also even, being given by

$$G(x) = G(k^2) = k \cot(\delta_0(k) + kR).$$ (2)

In a formal sense, this is the general case, since case (a) can be recovered by simply setting $R = 0$ and interpreting $G(x)$ as the scattering function previously designated by $F_l(x)$. Then, generally, the discrete function $G(x_j)$ is to be represented as a rational function.

Such problems as we describe here have been characterized by Miller as ill posed [21]. However, with sufficiently high quality data and proper constraints on the assumed rational form of $G(x)$ to assure vanishing phase shifts at high energies, there has been success in reproducing important features of models of the NN interaction [2, 4].

The meromorphic continuation of $G(x)$ can be characterized in statistical terms: Minimize the functional

$$\chi^2 = \sum_{j=1}^{N} [G_e(x_j) - G_t(x_j, \mathbf{a})]^2 / \sigma^2(x_j).$$ (3)

Given a set of data $\{G_e(x_j)\}$, associated standard errors $\{\sigma_G(x_j)\}$, and a theoretical function $G_t(x, \mathbf{a})$ depending upon a parameter vector $\mathbf{a}$, the value $\mathbf{a}_0$ which makes χ^2 an absolute minimum is sought. A special case is the least-squares problem, in which $\sigma_G(x_j) = 1$. Alternatively, standard errors $\{\sigma_\delta(x_j)\}$ for the phase shifts can be assumed at first, which are transformed into the set $\{\sigma_G(x_j)\}$. For the present analysis, it is also assumed that

$$G_t(x, \mathbf{a}) = P_L(x)/Q_M(x).$$ (4)

The right-hand side is often written simply as $[L/M]$, where L and M are the degrees of the polynomials $P_L(x)$ and $Q_M(x)$, whose coefficients are the parameters to be varied:

$$\begin{aligned} P_L(x) &= a_0 + a_1 x + \cdots + a_l x^L \\ Q_M(x) &= 1 + b_1 x + \cdots + b_M x^M. \end{aligned}$$ (5)

Two classes of problems need to be considered. We designate as class I a problem in which the data are smooth and the standard errors uniformly small. Often, in a class I problem, a simple analytic expression G_t is used to approximate a complicated analytical expression G_e. A contrasting situation occurs when data contain significant random variability. This is what we designate a class II problem. No one method we examine is superior for both classes of problems.

The context of the present work, then, is to find meromorphic approximations for the S matrix whose poles, zeros, and asymptotic behavior have physical meaning. Even though smooth functional fits to scatering data provided by inter-

polating and smoothing splines are well developed [16, 22], they do not satisfy the present requirements. This paper addresses the clear need for a comparable state of development for general rational functional data fits.

2. THREE STATISTICAL PADÉ APPROXIMANT METHODS

First we review some older methods. A rational approximant of the type described here is related to the Padé approximant (PA) [23]. Krasnopolsky *et al.* [9] refer to it as a Padé approximant of the third kind. Alternatively, it will be called a statistical PA. The standard PA, of the first kind, is possible when a power series of the function $G_e(x)$ is known. Then the coefficients in $P_L(x)$ and $Q_M(x)$ are simply and uniquely determined upon equating the power series for $G_e(x)$ and $P_L(x)/Q_M(x)$. Statistical PAs have sometimes been seen to provide a comparable quality of fits to PAs of the first kind [8, 24].

A second kind of PA that has seen some use in the past is the N point PA, one of many known generalizations of PAs [23]. It is determined by solving the equations

$$G_e(x_i)\,Q_M(x_i) = P_L(x_i), \qquad i = 1, 2, ..., L + M + 1 \qquad (6)$$

for $\{a_j\}$ and $\{b_k\}$. This is useful when data are known to high precision [9], but is frequently unstable even then, leading to defective PAs [3]. In a defective PA, common or nearly common roots of $P_L(x)$ and $Q_M(x)$ occur where the PA values should be smooth.

In general, any inappropriate occurrences of zeros or poles are to be regarded as defects. They can be anywhere in the complex plane. With careful scrutiny, it is usually possible to distinguish between defective poles and zeros and those that are not. For example, on mathematical grounds, zeros of $P_L(x)$ and $Q_M(x)$ that are identical to within the computational precision of the root-finding analysis should be regarded as defective. However, nearly common zeros of $P_L(x)$ and $Q_M(x)$ that are distinguishable within the computational precision sometimes are known to be approximations to cuts and can therefore be genuine [23]. A good example of this is seen in some recent calculations of S matrices in the complex k plane [8], in which the PA simulation of a cut appropriately approaches the imaginary axis (the Yukawa cut) as the cutoff radius R becomes larger [1]. As the identification of PA defects is important, and finding roots of polynomials is notoriously ill-conditioned [15], it is advisable to use extended precision in the procedure used to find roots.

Another mathematical ground for identifying defects is the occurrence of structure, such as poles, zeros, or oscillations, where it is known that none exist. For example, the phase shift $\delta_l(k)$ has no infinities in the physical region, where k is real and nonnegative. Finally, the physical significance of poles and zeros of a rational S matrix makes it possible to reject some otherwise excellent fits: Levinson's theorem [1, 5, 8], which allows one to compute the number of bound states from

the difference between the number of poles and zeros of the S matrix in the upper half plane, must be satisfied. Also, S matrix poles can represent bound states, antibound states, and resonances, and these features can be checked in the data or in the model being studied.

The first statistical PA method we present is a special case of a general meromorphic continuation of Miller's [21]. It is to minimize the functional χ_0^2:

$$\chi_0^2 = \sum_{j=1}^{N} [G_e(x_j) Q_M(x_j) - P_L(x_j)]^2 / \sigma^2 (x_j). \tag{7}$$

This does not give an absolute minimum of χ^2. Frequently, however, the fit is excellent. The equations to be solved are

$$\partial \chi_0^2 / \partial a_j = 0 \qquad j = 0, 1, ..., L$$
$$\partial \chi_0^2 / \partial b_k = 0 \qquad k = 1, ..., M. \tag{8}$$

These are linear in the $L + M + 1$ coefficients of P_L and Q_M. Although non-iterative, the Miller method is sometimes useful for providing a start of iterative methods.

The second statistical PA, the KKH algorithm, was introduced by Krasnopolsky, Kukulin, and Horáček [9]. They employed an iteration procedure which starts with the solution of Eqs. (8), which we call $P_L^{(0)}$ and $Q_M^{(0)}$. New standard errors are now defined:

$$\sigma_G^{(1)}(x_i) = \sigma_G(x_i) Q_M^{(0)}(x_i) \tag{9}$$

and Eqs. (8) are solved again. This linear process is iterated. The χ^2 functional, defined in terms of the original $\sigma_G(x_i)$, tends to decrease in a small number of iterations to a minumum value and then increase. The KKH procedure gives high weights to points near the poles, the zeros of $Q_M(x)$.

The third method, used by Hartt [3, 4] and discussed by Hartt and Yidana [8], called the HY method, is also linear and iterative. The original χ^2 of Eq. (3) is first minimized with respect to the $\{a_j\}$ keeping the $\{b_k\}$ fixed. This is obtained as the solution of the $L + 1$ linear equations

$$\partial \chi^2 / \partial a_j = 0 \qquad j = 0, 1, ..., L. \tag{10}$$

Next the reciprocal function $\{H_e(x_k) = 1/G_e(x_k)\}$ with reciprocal standard errors

$$\sigma_H(x_k) = \sigma_G(x_k) / |G_e^2(x_k) - \sigma_G^2(x_k)| \tag{11}$$

is used to form the functional

$$\chi_H^2 = \sum_{k=1}^{N} [H_e(x_k) - Q_M(x_k)/P_L(x_k)]^2 / \sigma_H^2(x_k) \tag{12}$$

which is minimized with respect to the $\{b_j\}$ from the solution of the M linear equations

$$\partial^2 \chi_H^2 / \partial b_k = 0, \qquad k = 1, 2, ..., M. \tag{13}$$

For each successive iteration, Eqs. (10) are solved and then Eqs. (13) are solved. Like the KKH method, the HY method tends to give χ^2 values which reach a minimum in a small number of iterations and then increase. Sometimes the Miller method gives good starting values for this iteration procedure, but as seen in the examples, it frequently does not.

3. Numerical Calculations

3.1. EXAMPLE 1. Our first example is a class I problem. It is to reconstruct the rational function $f_1(x) = (3 + 2x)/(1 + x/2)$. With the N point PA, we are restricted to three points for the three undetermined coefficients. As long as the values of $f_1(x_i)$ used as data are sufficiently different, solution of Eqs. (6) leads to accurate [1/1] coefficients. The statistical PAs allow the use of more data and generally improve as the number of data points increases. It is advisable to use high precision because polynomial roots are routinely calculated in the various PA checks, and much precision is lost because of the ill-conditioned nature of the root-finding problem. All calculations reported here have employed extended (32-figure) precision. There is a wide range of results if $f_1(x)$ is calculated at only four values of x. With the choice $(-2.25, -1.75, -1, +1)$, for example, the Miller method gives coefficients with better than 25-figure accuracy and $\chi^2 = 10^{-61}$, making further iterations using the KKH method superfluous. The HY method is ineffective and does not converge even after hundreds of iterations, unless the starting values are close to the exact ones. As the number of data points of $f_1(x)$ is increased, the convergence of the HY method dramatically improves. With just 10 points judiciously chosen, the HY method converges to $\chi^2 = 10^{-18}$ and ten-figure accuracy after 9 iterations, starting from $a_0 = a_1 = 0 = b_1$. Again, the Miller method gives essentially exact results. It is more realistic to use more data points. Fitting a small number of data points can equally well be accomplished by many different low-order PAs and hence is an ill-posed problem.

3.2. EXAMPLE 2. The second example is a classic nuclear scattering problem. It is to construct a rational S matrix in the neutron-proton singlet s wave channel. The analysis is carried out here using data in the form of phase shifts, according to the prescription of case (a) in which R is set equal to zero. In this and the next example, smooth and noisy data are considered in succession. Some older smoothed phase shifts and associated standard errors are especially easy to use here [4, 25]. We use 40 data points. Figure 1 shows the curve for our best statistical fit, expressed in terms of phase shifts that have been transformed from our [3/2] fit of
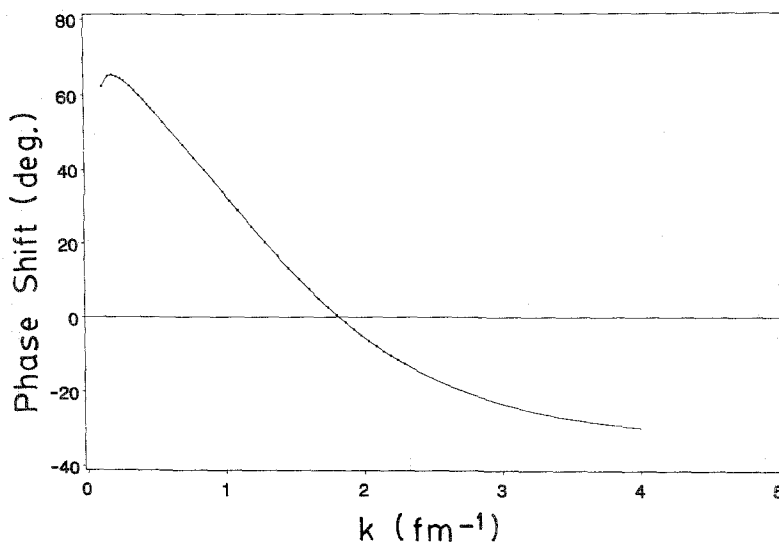
FIG. 1.   Neutron–proton $^1S_0$ phase shifts. Shown are experimental data points $(\cdot)$ [4, 25] and curve generated from KKH method [3/2] fit of scattering function $F(x) = k \cot(\delta)$.

the scattering function. The original experimental phase shifts [25], obtained by an energy-dependent smoothing procedure, are also shown. The curve was obtained using the KKH method, which gave $\chi^2 = 0.0356$ after 2 iterations, and the parameters (rounded off):

$$a_0 = 0.04224044227 \text{ fm}^{-1} \qquad b_1 = 1.538415449 \text{ fm}^2$$

$$a_1 = 1.319236280 \text{ fm} \qquad\qquad b_2 = -0.5557873921 \text{ fm}^4$$

$$a_2 = 1.588550849 \text{ fm}^3$$

$$a_3 = 0.09624740411 \text{ fm}^5$$

Fitting such smooth data is a class I problem. The KKH method is slightly better here than the HY method, which took five iterations to reach $\chi^2 = 0.0359$, with an identical phase shift curve. The Miller method gave $\chi^2 = 0.174$, also a good fit, and provided the start of all the iterative methods for this example. The NR method gave $\chi^2 = 0.0356$ after five iterations, while the LM method gave $\chi^2 = 0.0357$ after 10 iterations. Generally, fits to $G(x)$ of the form $[L/M]$ with $M < L$ are needed to reproduce the correct asymptotic behavior of the phase shifts—they vanish—as k approaches infinity, for a finite or a Yukawa-type potential [4].

It is also a class I problem to reconstruct the [3/2] PA. With the [3/2] coefficients given above and the experimental standard errors for 40 data points, the Miller method reproduces $F(k)$ with $\chi^2 = 10^{-55}$. The HY, LM, and NR methods, all more complicated and time consuming than the Miller method, have not been

tested here. The Miller method also produces good [2/1], [4/3], and [5/4] fits. The [4/3] and [5/4] fits are defective and hence are rejected.

3.3. EXAMPLE 3. The situation changes when some random error is built into the phase shift data, throwing the problem into the second class. For a numerical experiment, we have folded Gaussian noise consistent with the experimental standard errors into the 40 data points, using an IMSL random number generator [16]. Figure 2 shows randomly generated phase shift data in the region of largest standard errors. For the original data here, we have taken the theoretical phase shifts from the [3/2] fit shown in Fig. 1. Two cases are shown, corresponding to two different values of the IMSL random number parameter DSEED. At lower energies the variability is less, standard errors increasing smoothly with k from $0.01°$ to $1.74°$ [25]. Table I gives the results for convergence comparisons. Here it is evident that the HY method displays the best convergence. A second example is shown in Table II, where Gaussian noise is introduced corresponding to values of $\sigma(x_j)$ reduced by a factor of 0.5. Comparison of these tables indicates a relative improvement of the KKH method when data have smaller statistical variability. Note that the NR and LM methods are inferior in both cases, often not converging when the Miller method provides the starting values.

Especially over the lower energies, the noise we have generated perturbs the data only slightly; yet, it is not possible to recover the [3/2] order of the original theoretical data, either in Table I or Table II, by the χ^2 fits alone. Some other
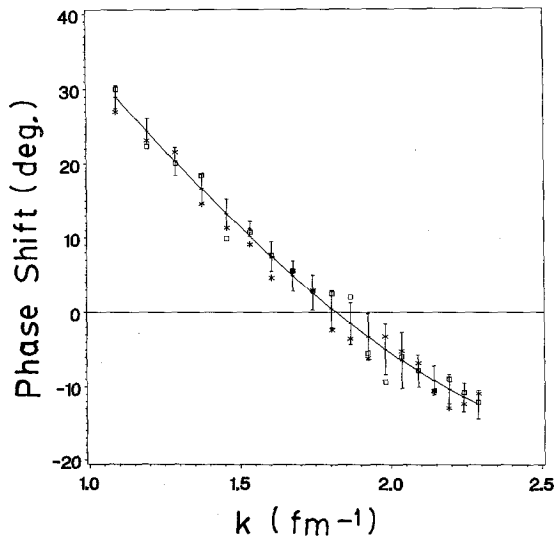

FIG. 2. Neutron–proton $^1S_0$ phase shifts in region of large standard errors. Shown are experimental error bars [25] and phase shifts obtained by perturbing fit shown in Fig. 1 with Gaussian random error. Gaussian standard deviation was set equal to standard error. Two cases are shown, corresponding to IMSL [16] random number parameter DSEED = 1 (+), and DSEED = 20 (□).

TABLE I

Values of χ^2 for Different Methods of Fitting $G(x)$ with Random Variability in Data

		Methods				
PA	DSEED	Miller	KKH	HY	NR	LM[c]
[2/1]	1	92.0 L	71.1(2) L	93.6(2)[a] L	69.9(4) L	70.32 L
	20	87.7 L	87.7(1) L	419(4)[a] L	82.6(2) L	83.5 L
[3/2]	1	713 D	124(3) D	35.8(5)[a] D	[b]	[b]
	20	539 D	119(3) D, L	40.7(4)[a]	[b]	[b]
[4/3]	1	523 D, L	107(2) D, L	28.2(6)[a] D, L	423(1) D, L	45.0 D
	20	0.19 + 7 D, L	68.2(2) D, L	33.0(4)[a] D, L	[b]	103 D, L
[5/4]	1	988 D	116(3) D, L	26.3(4)[a] D	[b]	[b]
	20	0.28 + 4 D, L	156(2) D, L	28.0(3)[a] D, L	[b]	878 D, L

Note. Data are from the KKH method [3/2] fit of Fig. 1, folded in with Gaussian random variations, as shown in Fig. 2, generated with standard deviations equal to experimentl standard errors. The number of iterations to reach a minimum χ^2 is in parentheses. D denotes a defective PA. L denotes a PA that does not satisfy Levinson's theorem. DSEED is the IMSL [16] random number parameter.

[a] In these cases, the χ^2 is significantly improved using the starting values $a_1 = b_1 = 1$, all others $= 0$, rather than those given by the Miller method.

[b] The method fails to converge for either the Miller starting values or those of footnote *a*.

[c] For the LM method, 25 iterations were used in all cases, giving χ^2 convergence to 3 significant figures.

TABLE II

Values of χ^2 for Different Methods of Fitting $G(x)$ with Reduced Random Variability in Data

		Methods				
PA	DSEED	Miller	KKH	HY	NR	LM[c]
[2/1]	1	520 L	90.3(2) L	87.5(3)[a] L	59.6(6) L	60.1 L
	20	79.5 L	71.0(2) L	96.4(2)[a] L	65.2(5) L	66.0 L
[3/2]	1	18.0	13.3(2)	12.1(1)	8.14(5)	8.13
	20	168	80.0(4) D	16.7(10)	[b]	27.9
[4/3]	1	0.35 + 5 D, L	81.1(3) D, L	11.5(2)[a] D, L	[b]	26.1 D, L
	20	192 D, L	9.7(2) D, L	7.69(10) D, L	[b]	32.0 D, L
[5/4]	1	0.58 + 3 D	11.1(2) D	6.96(5)[a] D	[b]	[b]
	20	95.1 D	47.1(3) D	7.73(10)[a]	95.3(1) D	[b]

Note. This is the same as Table I except that the standard deviations of the random variatons have been reduced by half.

[a] In these cases, the χ^2 is significantly improved using the starting values $a_1 = b_1 = 1$; all others $= 0$, rather than those given by the Miller method.

[b] The method fails to converge for either the Miller starting values or those of footnote *a*.

[c] For the LM method, 25 iterations were used in all cases, giving χ^2 convergence to 3 significant figures.

criteria must be applied here that rule out most of the solutions. First, in this analysis it is necessary to have an on-line root finder that factors $P_L(x)$ and $Q_M(x)$ in order to detect defective PAs. Our root finder, using the Bairstow (i.e., Newton–Raphson) method, has helped identify numerous defective fits. They are labeled "D" in the tables. Second, a physical constraint here is that there are no np $^1S_0$ bound states. Consequently, by Levinson's theorem, $\delta(0) = \delta(\infty)$ [1]. To check this, we have found it convenient to calculate and factor the S matrix, which in the s wave is

$$S(k) = \frac{P_L(k^2) + ikQ_M(k^2)}{P_L(k^2) - ikQ_M(k^2)}. \tag{14}$$

For Levinson's theorem to be satisfied when there are no bound states, the number of poles of $S(k)$ in the upper and lower half-planes must be equal [1, 5]. Fits that do not satisfy Levinson's theorem are labeled "L" in the tables. In Table I, there are no physically acceptable fits for DSEED = 1, while for DSEED = 20 there is only one, given by the HY method, which recovers the [3/2] order of the PA. Even with a smaller random variability in the data, as in Table II, the [3/2] order is recovered as the only physical acceptable solution; and here, again, the HY method is clearly the best.

3.4. EXAMPLE 4. Gamow state (resonance) poles are calculated here for some central NN potentials using the methods under discussion. Since a cutoff radius R for the potentials is explicitly introduced in order to produce S matrix poles for our Yukawa-type potentials, the prescription for case (b) is applied here. As the data to be fitted are theoretical and of high precision, this is a class I problem. The KKH method is the best for this and converges after two iterations to stable locations of these poles. The number of such poles allows an estimate of the rank of a separable expansion required up to some fixed high momentum limit k_{max} [10, 13]. In recent work, stable, accurate results have been found for the Malfliet–Tjon spin-averaged np potential V (MTV) [10, 26] and the $^1S_0$ Reid soft core potential [11, 24]. Here, the truncation range R is set, accurate phase shifts (typically on the order of 100) are computed using the summed Noumerov method [8, 27], and χ^2 is minimized. Figure 3 shows a plot of results for the MTV potential in the present case, where we choose $R = 5$ and 6 fm. Finding Gamow poles is the most spectacular success of the KKH method we have seen, as it eliminates the need to solve a difficult eigenvalue problem if only the location of the Gamow states is needed.

We have always been able to find approximate S matrices that, for a given k_{max}: (a) satisfy Levinson's theorem and (b) also have well-converged Gamow poles. Such S matrices are good candidates for use in inverse scattering theory. In practice, however, we find that for every k_{max} there is a maximum order of the PA for $G(k)$ for which Levinson's theorem is satisfied. When constraints (a) and (b) are both satisfied, the S matrices give correct poles and phase shifts only up to $k \approx k_{max} - 1\,\text{fm}^{-1}$. It is important to note that even with this limitation, the statistical PA methods we present here are considerably more powerful than classical PAs based on effective range expansions [8].
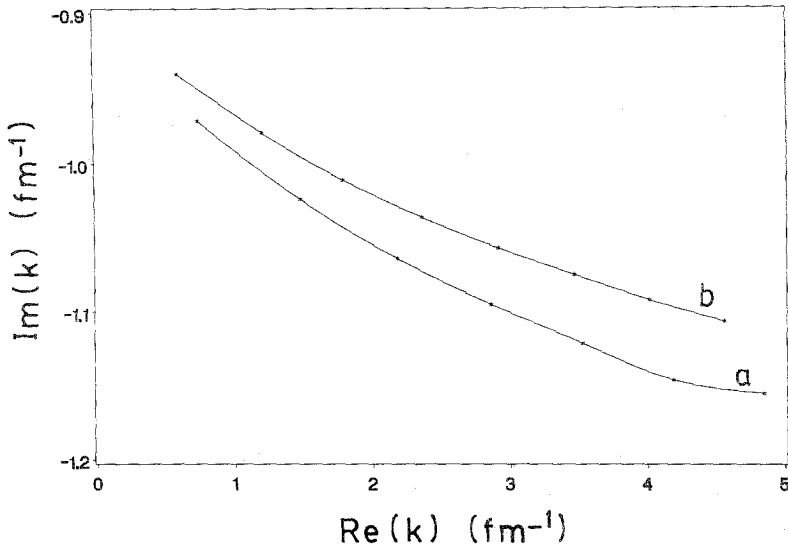
FIG. 3. Poles of S matrix of the Malfliet–Tjon potential V obtained from [21/20] fit to $G(k)$ at $R = 5$ fm (a) and $R = 6$ fm (b).

3.5. EXAMPLE 5. The HY method can easily be adapted to the use of linear constraints on the solutions. For example, the scattering length a and effective range r_0 can be known more accurately than the phase shifts. These are the first two terms in the effective range expansion of $G(x)$, where again we have set $R = 0$ in Eq. (2):

$$G(x) = -\frac{1}{a} + \frac{1}{2} r_0 x - r_0^3 P x^2 + \cdots. \tag{15}$$

Fits to $G(x)$ are constrained to reproduce given values of a and r_0 provided the PA coefficients satisfy

$$a_0 = -\frac{1}{a}, \qquad a_1 - a_0 b_1 = \frac{1}{2} r_0.$$

These equations can be used as constraints on a_0 and a_1 in the first half of the iteration, when a fixed value of b_1 is assumed. Consider our [3/2] solution with the quoted coefficients, again. It gives $a = -23.673995$ fm and $r_0 = 2.5085059$ fm, while for DSEED = 1 the [3/2] fit of Table II gives $a = -23.592961$ fm and $r_0 = 2.4787987$ fm, with $\chi^2 = 12.1$. Our fit that is constrained to the original (exact) values of a and r_0 gives an almost equally good fit, with $\chi^2 = 12.3$.

4. CONCLUSION

There is a spectrum of problems ranging between class I and class II in which superior convergence is alternatively obtained by the Miller, KKH, and HHY

methods. Although the derivative matrix M_{ij} is easily calculated, this amounts to extra effort required with the use of the Newton–Raphson method, and as we see, the NR method generally displays inferior convergence or even nonconvergence. The LM method, easy to use with available programs, also fails or converges slowly in many cases. The existence of noise in the data strongly favors the use of the HY method. With noisy data, converged HY results are sometimes slightly improved with further NR or LM iteration. We recommend all five statistical Padé methods be programmed together as options whenever rational function fits of experimental scattering data are sought.

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