Padé Approximants, NN Scattering, and Hard Core Repulsions

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Padé approximants to the scattering function $F = k \cot(\delta_0)$ are studied in terms of the variable $x = k^2$, using four examples of potential models which possess features of the np $^1S_0$ state. Strategies are thereby developed for analytically continuing F when only approximate partial knowledge of F is available. Results are characterized by high accuracy of interpolation. It is suggested that a physically realistic inverse scattering problem begins with such an analytically continued F. When it exists, the solution of this problem in terms of the Marchenko equation is a local potential of the Bargmann type. Some strategies for carrying out this program lead to a stably defined potential, while others do not. With hard core repulsions present, low order Padé approximants accurately describe F for $E_{c.m.} \leq 300$ MeV. However, since the condition $\delta(\infty) - \delta(0) = 0$ is not satisfied in any of our examples containing hard core repulsions, the Marchenko method does not have a solution for them. A possible physical consequence of this result is discussed. Another inverse scattering method is proposed for application to hard core problems.

> NUCLEAR REACTIONS Padé approximants used to calculate $k \cot(\delta_0)$ and to solve inverse scattering problem for models of np $^1S_0$ scattering; effects of hard cores.

I. INTRODUCTION

A goal in nuclear physics is to describe the interaction between nucleons in agreement with experiments and underlying dynamical principles.[1] Phenomenologies used in attaining accurate fits of nucleon and meson scattering data are elements in achieving this goal. Recent developments employing dispersion relations for two pion exchange have led to two new meson-theoretic potential models of the nonrelativistic NN interaction.[2] While one of these potentials has no free parameters,[3] the other is semiphenomenological in that a short-range repulsion is introduced to fit phase shifts derived from experiment.[4] Other more phenomenological potential models have also been developed in recent years which have introduced unusually weak short-range repulsions, referred to as super soft cores (SSC),[5] designed to give excellent agreement with np $^1S_0$ and other low angular momentum phase shifts.[6] With one pion exchange effects having been successfully included and evaluated through an NN phase shift analysis,[6] efforts are underway to include both vector and pseudoscalar meson exchange effects in future analyses.[2] Phenomenology and meson-theoretic approaches are thus seen to be drawing closer together, each using some parts of the other. Clearly, high interest continues in refining phenomenological techniques for studying the two-nucleon interaction.[7]

Padé approximants (PA)[8] have a possible role in scattering phenomenology; their use in low and medium energy NN scattering is the subject of this paper. A PA is a ratio of polynomials defined to have the same truncated Taylor series as the function it represents. For theorems and conjectures about the convergence and analytic continuation properties of a PA the reader is referred to Baker.[8] An additional problem of uniqueness arises when the Taylor series is not known, as in fitting experimental data, and methods of approximating a PA must be used. We introduce techniques useful in fitting data and study uniqueness of interpolation using different approximation criteria by making comparisons with known functions. Our computational framework is given in Sec. II.

The scattering function studied here is $k \cot(\delta_0)$, where k is the relative momentum and δ_0 is the s-wave phase shift. Reference in the sequel is made to this function as $F(x)$, expressed in terms of the variable $x = k^2$, which is proportional to the energy $E_{c.m.}$ in the center of mass system when $E_{c.m.}$ is nonrelativistically defined. Four examples are chosen which are appropriate to the simple and much-studied experimental situation, the np $^1S_0$ state. A two-fold problem is considered: Given a partial knowledge of the scattering function of a given potential, (1) find its appropriate Padé approximants and (2) use the Padé approximants to construct approximations to the original potential.

We study four local potential models for which the scattering function can be computed to high numerical precision. These are the hard core (HC), square well (SW), hard core square well (HCSW), and hard core Yukawa (HCY). Data generated using these model potentials are fitted in this investigation to learn how well the procedures

work under verifiable conditions. A subsequent study employing the full range of np $^1S_0$ phase shifts obtained by MAW is reported elsewhere.[9]

Knowledge of the effective range expansion, given by

$$k \cot(\delta_0) = -\frac{1}{a} + \frac{r_0}{2}k^2 - Pr_0^3k^4 + Qr_0^5k^6 + \cdots$$

(1.1)

is central to the first problem in that it either leads to Padé approximants or is computable from them. In contrast to np scattering experiments, from which only the scattering length a and the effective range r_0 are reliably known for the $^1S_0$ state,[10] three of our model potentials can be used to generate analytic expressions for the shape parameter P and higher terms. Furthermore, as reviewed in Sec. III, the presence of a hard core can also be managed by analytical procedures. As pointed out in the Discussion, an analytical Padé hard core transformation introduced in Sec. III may have some applications to both of the problems posed above.

The second problem, which is to recover a local potential from Padé approximants to $F(x)$, can be considered a "physical inverse scattering problem," in that realistic experimental physical conditions in determining $F(x)$ are assumed. Only partial knowledge of $F(x)$ over a finite energy range is used in obtaining an analytic form of $F(x)$ produced in an approximate analytic continuation of the effective range expansion. A local potential is then generated which exactly reproduces the analytically defined scattering function. In contrast, a corresponding "mathematical inverse scattering problem" either starts with complete knowledge of the phase shifts of a single partial wave at all energies, or the phase shifts of all partial waves at one energy, from which a local potential is derived.[11]

Given the scattering function $F(x)$ in Padé form, the inverse problem is quickly and easily solved by the integral equation procedure of Marchenko,[12] provided that it is possible to be solved. The case at hand, the np $^1S_0$ state, is simple in that there are no bound states, and therefore any solution is unique.[12] Lambert, Corbella, and Thomé have shown[13] that the necessary and sufficient condition for solvability of this inverse scattering problem is

$$\delta(\infty) - \delta(0) = 0 \qquad (1.2)$$

whenever the scattering function has the form

$$F(x) = \frac{P_L(x)}{Q_M(x)} \equiv [L/M], \qquad (1.3)$$

where L and M are the degrees of the numerator and denominator polynomials, and provided that $M \leq L - 1$. It is easily seen that a hard core repulsion by itself cannot satisfy the conditions of this theorem because Levinson's theorem does not apply to such a case.

The condition Eq. (1.2) is easily checked. We shall not display any of the potentials which result from the solution of the inversion problem, remaining content in this paper to see whether Eq. (1.2) is satisfied in various cases. Some details of the Marchenko procedure are given in the paper by Sprung and Srivastava wherein the first SSC potential model is developed starting from the MAW phase shifts.[14] A reanalysis of the MAW data, based in part upon the results of this paper, but made along lines similar to Ref. 14, is presented elsewhere.[9]

There are questions about the stability of various approaches to the physical inverse scattering problem. Can a convergent procedure be found that is relatively insensitive to incomplete knowledge of the phase shifts, especially at high energies? LCT studied examples which appeared stable with respect to small variations of the effective range parameters. However, Viano found instabilities to be inherent in the inversion problem which starts with phase shifts at a fixed energy.[15] An efficient computational algorithm for minimizing χ^2, called MINIRAT, has recently been developed especially for rational functions.[16] The convergence of the iterated Padé parameters for the examples of this paper together with the Padé fit of $F(x)$ using MINIRAT are evidence of stability. Another technique commonly used is applied and is seen to exhibit a type of instability, as defined in the next section. Section IV gives the results of these computations.

In the Discussion (Sec. V), a shortcoming of our approach to the inverse scattering problem for potentials containing hard core repulsions is pointed out, a conjecture is made about a possible physical consequence, and a method is proposed for application to hard core problems.

II. PADÉ METHODS

Consider a function $f(x)$ which is to be represented by the rational approximant $P_L(x)/Q_M(x)$, where $P_L(x)$ and $Q_M(x)$ are polynomials of degree L and M. The Padé algorithm is to expand $f(x)$ as a power series, $f(x) = \sum_{r=0}^{\infty} C_r x^r$, and to solve the linear equations resulting from equating coefficients of powers of x in

$$Q_M(x)f(x) = P_L(x) + O(x^{L+M+1}). \qquad (2.1)$$

The coefficients in $P_L(x)$ and $Q_M(x)$,

$$P_L(x) = \sum_{s=0}^{L} a_s x^s, \tag{2.2a}$$

$$Q_M(x) = \sum_{t=0}^{M} b_t x^t, \tag{2.2b}$$

are determined in this way. Setting $b_0 = 1$ normalizes P and Q. The solution, written as $[L/M]$, has the same power series as $f(x)$ through the first $L + M + 1$ terms. Through the use of powerful recursion algorithms, $[L/M]$ can be used to generate a table of other Padé approximants (PA).[8]

In the current application we are exclusively concerned with the scattering function $F(x)$ $= k \cot(\delta_0)$. From experiments, $F(x)$ is determined numerically at a discrete set of N energies and a goal can be to construct a Taylor series, which is just the effective range expansion, from these data. A more ambitious goal is to construct Padé approximants directly. Originally formulated and solved as a classical interpolation problem by Cauchy, the latter problem has seen refinements by a succession of workers.[8] Following Baker, we refer to solutions as N-point Padé approximants (NPA). Different means of determining NPA have been explored and important applications have already been made to scattering problems, as discussed by Haymaker and Schlessinger.[17] They employed NPA for analytically continuing scattering functions from a mathematically accessible but unphysical region of momenta to the physical region.

HS illustrated the superiority of point methods over norm and moment methods in their NPA calculations. A simple and straightforward point method which we also employ is to solve the linear equations

$$P_L(x_k) f(x_k) = Q_M(x_k), \quad k = 1, 2, \ldots, L + M + 1 \tag{2.3}$$

for the coefficients in $P_L(x)$ and $Q_M(x)$. The rational function approximant fits $f(x)$ precisely at the $L + M + 1$ points used. Although this procedure should be appropriate when $f(x)$ itself is known with great precision, to force a precise fit to a function only known approximately from experiment can lead to poor fits, including unwanted poles and zeros, in regions where f is known but its values are not among the $L + M + 1$ data points used. Rational approximants possessing such unwanted poles and zeros are termed defective. As seen in Sec. IV, defective NPA are often generated even when the data are given with high precision. This is easily understood. The ansatz

that the scattering function $F(x)$ has a particular rational form must generally be regarded as an approximation, albeit in many cases a very good one.

Defective NPA are sometimes useful for interpolation; however, they are unacceptable for solving the inverse scattering problem. If an inverse scattering method produces defective NPA as a recurring artifact which is sensitive to small changes in the data, then that method must be considered to exhibit instability.

Another point method to find the NPA to a scattering function is to determine $P_L(x)$ and $Q_M(x)$ either by least squares or χ^2 minimization. These have the advantages of norm methods[17] in fitting approximate data approximately, and including all data. The use in this paper of the χ^2-minimization procedure, MINIRAT,[16] appears to be free of defects that occur in the exact N-point fits. This is shown in the numerical results in Sec. IV.

A variety of rational approximants is tested in this paper. We now introduce a compact notation for distinguishing them. The symbol $[L/M]$ refers to a Padé approximant determined from a Taylor series, while $[L/M]_t$ is an approximant obtained by truncating both numerator and denominator of a representation of a function given as a ratio of two infinite series. While the latter $[L/M]_t$ is clearly not a PA it can be used to find a PA. An exact fit to $L + M + 1$ points is denoted by $[L/M]_n$, and $[L/M]_c$ is either a minimum χ^2 or a least-squares fit.

The values of L and M used for this paper are restricted to $L = M + 1$, which satisfies a condition in the LCT theorem[13] on the solvability of the inverse scattering problem. This choice of L and M also gives the same asymptotic behavior of $F(x)$ at high energy as the Born approximation of a Yukawa potential. Experience has shown[18] that for $E_{c.m.} \lesssim 300$ MeV, the condition $L = M + 1$ appears to be optimal for strictly attractive short-range potentials, while in the presence of short-range repulsions, scattering functions are nearly equally well fitted when the conditions $L = M$ or $L = M - 1$ are satisfied. For a hard core potential, $F(x)$ does not display asymptotic convergence, with zeros and poles alternating over all positive energies. However, the asymptotic form $F(x) \sim x$ is a reasonable requirement upon $F(x)$ when the fit is over a finite energy range and the potential is attractive with an inner hard core repulsion.

III. ANALYTIC EFFECTIVE RANGE EXPANSIONS

Our calculations are based upon solutions of the s-wave Schrödinger equation

$$\frac{d^2u}{dr^2} + (k^2 - U)u = 0, \tag{3.1}$$

where $k^2 = 2\mu E/\hbar^2$ and $U = 2\mu V(r)/\hbar^2$. Natural units ($\hbar = c = 1$) are used. The reduced np mass is used for μ, and for computational convenience two fundamental constants are defined and used throughout. They are a reduced Compton wavelength $\hbar/2\mu c = 0.210\,164\,17$ fm, and a conversion factor 1 MeV $= 5.067\,689\,3 \times 10^{-3}$ fm^{-1}. These are consistent with a recent revision of physical constants.[19]

A. Hard core

Since hard cores have seen much use in NN potential models and are simple to study, they are our first example. The s-wave phase shift is simply $-kR$, where R is the hard core radius and the scattering function $F(x) = k \cot(\delta_0)$ occurs naturally as a ratio of two infinite series in the variable $x = k^2$:

$$F(x) = -\frac{\cos(kR)}{(1/k)[\sin(kR)]}. \tag{3.2}$$

The first few terms of the Taylor series are needed:

$$F(x) = -\frac{1}{R}\left(1 - \frac{R^2}{3}x - \frac{R^4}{45}x^2 - \frac{2R^6}{945}x^3 - \frac{R^8}{4725}x^4 - \cdots\right). \tag{3.3}$$

Of the strategies mentioned in Sec. II, truncation, PA, and NPA (except for χ^2 minimization and least squares) are used both in this example and for the square well.

B. Square well

For scattering by a square well of radius b and well depth V_0, the scattering function takes the form $F(x) = N/D$, where

$$N = k \sin(Kb) + K \cos(kb)\cos(Kb), \tag{3.3a}$$

$$D = \sin(Kb)\cos(Kb) - \frac{K}{k}\sin(kb)\cos(Kb), \tag{3.3b}$$

with

$$K = (k_0^2 + k^2)^{1/2} \text{ and } k_0 = (2\mu V_0)^{1/2}.$$

The expansion of N and D in powers of x is given in terms of the coefficients in $N = \sum N_r x^r$ and $D = \sum D_r x^r$, where we also introduce $S = \sin(k_0 b)$ and $C = \cos(k_0 b)$ in giving the terms used in the present work:

$$N_0 = k_0 C,$$

$$N_1 = S\left(\frac{b}{2}\right) + C\left(\frac{1}{2k_0} - \frac{b^2 k_0}{2}\right),$$

$$N_2 = S\left(\frac{b^3}{12} - \frac{b}{8k_0^2}\right) + C\left(\frac{k_0 b^4}{24} + \frac{b^2}{8k_0} - \frac{1}{8k_0^3}\right),$$

$$N_3 = S\left(-\frac{b^5}{80} - \frac{b^3}{24k_0^2} + \frac{b}{16k_0^4}\right)$$
$$+ C\left(-\frac{b^6 k_0}{720} - \frac{b^2}{16k_0^3} + \frac{1}{16k_0^5}\right), \tag{3.4}$$

$$N_4 = S\left(\frac{b^7}{2016} + \frac{b^5}{192k_0^2} + \frac{5b^3}{192k_0^4} - \frac{5b}{128k_0^6}\right)$$
$$+ C\left(\frac{k_0 b^8}{403\,20} - \frac{b^6}{576k_0} - \frac{b^4}{384k_0^3}\right.$$
$$\left. + \frac{5b^2}{128k_0^5} - \frac{5}{128k_0^7}\right),$$

and

$$D_0 = S - Ck_0 b,$$

$$D_1 = C\frac{b^3 k_0}{6},$$

$$D_2 = -S\left(\frac{b^4}{24}\right) + C\left(-\frac{b^5 k_0}{120} - \frac{b^3}{24k_0}\right), \tag{3.5}$$

$$D_3 = S\left(\frac{b^4}{48k_0^2} + \frac{b^6}{360}\right) + C\left(\frac{b^3}{48k_0^3} - \frac{b^5}{240k_0} + \frac{b^7 k_0}{5046}\right).$$

These are sufficient to obtain the first four terms of the effective range expansion and to evaluate [2/1].

C. Hard core Padé transformation

If a potential $V(r)$ gives rise to a phase shift $\delta_0(k)$, then the potential $V(r - R)$ outside a hard core of radius R is easily seen to produce a phase shift of $\delta_0(k) - kR$. This relationship between the two phase shifts has a counterpart in Padé phenomenology. If the original potential $V(r)$ gives the scattering function $F = N/D$, it follows that the new potential $V(r - R)$, plus hard core of radius R, has the solution $\overline{F} = \overline{N}/\overline{D}$ with

$$\overline{N} = N + [k \tan(kR)]D, \tag{3.6a}$$

$$\overline{D} = D - N\frac{\tan(kR)}{k}. \tag{3.6b}$$

If N/D is a Padé approximant and a Taylor series is used for $\tan(kR)$, then a rational function is obtained by truncating $\overline{N}$ and $\overline{D}$. This function is of course not a Padé approximant. The Padé procedure is to use $\overline{N}/\overline{D}$ to generate $L + M + 1$ terms of the effective range expansion, from which $[L/M]$ is found. The terms in this series are easily obtained, although their complexity rapidly grows. We give transforma-

tions here for the first three effective range parameters a', r_0', and P' in terms of a, r_0, and P obtained from $V(r)$:

$$a' = a + R, \tag{3.7a}$$

$$r_0' = r_0/y^2 + 2R/y + 2R^3/(3a^2y^2), \tag{3.7b}$$

$$P'(r_0')^3 = Pr_0^2/y^2 - R^6/(45a^3y^3) - 2R^5/(15a^2y^3)$$
$$- R^4/(3ay^3) - R^3 r_0/(6ay^3) - R^3/(3y^3)$$
$$- R^2 r_0/(2y^3) - R r_0^2/(4y^3), \tag{3.7c}$$

where $y = 1 + R/a$. It is useful to be able to find the effective range parameters (a, r_0, P) associated with $V(r)$ in terms of experimental values (a', r_0', P') and R. By the symmetry of the problem, this transformation is obtained by making the interchanges in Eqs. (3.7):

$$(a, r_0, P, R) \rightarrow (a', r_0', P', - R). \tag{3.8}$$

IV. COMPUTATIONS

In the examples that follow, we employ several sets of energies for evaluating the NPA. The subscript i in $[L/M]_{ni}$ denotes that choice:

$i = 1$: $E_n = n$ MeV, $n = 1, 2, \ldots$,

$i = 2$: $E_n = 5n$ MeV, $n = 1, 2, \ldots$,

$i = 3$: $E_n = 0.5n - 0.25$ MeV, $n = 1, 2, \ldots$,

$i = 4$: $E_n = 2n - 1.75$ MeV, $n = 1, 2, \ldots$,

$i = 5$: $E_n = 14n - 13.75$ MeV, $n = 1, 2, \ldots$.

We have not formulated a precise criterion for an optimal energy set. However, experience suggests a compromise between low energies, which are superior for effective range parameters, and a large energy spread, which tends to produce fewer defects.

We also consider two different cases of the use of MINIRAT in χ^2 minimization: $j = 6$ or 7 in $[L/M]_{cj}$. For $j = 6$, the scattering function is evaluated at the 40 energies used by MAW in their solution for the np $^1S_0$ phase shifts and their standard errors are also employed in the χ^2 functional.

For $j = 7$, the same energies are used as for $j = 6$, but the standard error (in the phase shifts) is held constant at 0.01 degrees. In effect, the $j = 7$ case is a least-squares fit of the phase shifts. For $j = 8$, the procedure is identical to $j = 6$ except that only the lowest 24 energies are used (through $E_{c.m.}$ $\lesssim 70$ MeV.

A. Hard core

We fix the value of the hard core radius at 0.5 fm. Then the singularities in $F(x)$ are simple poles at $k = 2n\pi$ fm^{-1}, $n = 1, 2, \ldots$, even the first occurring at a relativistic energy beyond the physical region of validity of this nonrelativistic model. However, the problem is mathematically well defined and convergence to the first pole is a test of the NPA.

Table I gives the coefficients of various rational approximants and Table II compares the different locations of the first pole. When the exact expression for $F(x)$, given in Eq. (3.2), is simply truncated, the location of the pole is clearly inferior to the values given by $[L/L - 1]$ and $[L/L - 1]_n$. For $[3/2]_t$ there is no pole. The $[L/L - 1]_n$ results closely resemble those for $[L/L - 1]$ when care is taken to fit points over a sufficiently large energy range. There is excellent numerical agreement among all the approximations considered in the medium energy range ($k \lesssim 3$ fm^{-1}). A 0.1 percent numerical precision is achieved by all approximations considered, with the exception of $[2/1]_t$.

B. Square well

The well depth V_0 and range b of our SW model have been chosen to fit the experimental np singlet scattering length, $a = -23.719 \pm 0.013$ fm, and effective range $r_0 = 2.76 \pm 0.05$ fm.[10] They are $b = 2.640\,967\,2$ fm and $V_0 = 13.455\,115$ MeV. Table III gives the parameters of the scattering function for various approximations and Table IV displays values of $F(x)$ for these same approximations.

From $[4/3]_t$, with eight parameters, the first

TABLE I. HC Padé coefficients for $R = 0.5$ fm.

Approximation	a_1 fm^{-1}	a_2 fm^{-3}	a_3 (10^{-2}) fm^{-5}	a_4 (10^{-4}) fm^{-7}	b_2 (10^{-1}) fm^{-2}	b_3 (10^{-3}) fm^{-4}
$[3/2]_t$	−2	0.25	−0.5208	0.4340	−0.4167	0.5208
$[3/2]$	−2	0.2273	−0.2525	0.0301	−0.3030	0.1263
$[2/1]$	−2	0.2143	−0.1190		−0.2381	
$[3/2]_{n1}$	−2	0.2423	−0.4133	0.1195	−0.0038	0.3050
$[3/2]_{n2}$	−2	0.2273	−0.2526	0.0301	−0.3031	0.1264
$[2/1]_{n1}$	−2	0.2143	−0.1192		−0.2382	
$[2/1]_{n2}$	−2	0.2144	−0.1196		−0.2384	

TABLE II. Location of first pole for HC potential with $R = 0.5$ fm.

Method	k (fm⁻¹)	error (%)
Exact	6.283	
$[4/3]_t$	6.034	−4.0
$[3/2]_t$ [a]		
$[2/1]_t$	3.820	−39
$[3/2]$	6.285	+0.029
$[2/1]$	6.481	+3.1
$[3/2]_{n1}$	6.186	−1.6
$[3/2]_{n2}$	6.285	+0.029
$[2/1]_{n1}$	6.480	+3.1
$[2/1]_{n2}$	6.476	+3.1

[a] No real pole occurs in this approximation.

four terms of the effective range expansion can be found. The PA, $[2/1]$, constructed from these four terms is clearly superior in reproducing $F(x)$. This illustrates the optimal property of the Padé method.

Truncation is not a unique procedure. If Eqs. (3.3) are divided by $\cos(kb)\cos(Kb)$ and the resulting rational function is truncated to $[4/3]$ the same effective range expansion to four terms results, but the errors in $F(x)$ grow rapidly with energy, order-of-magnitude discrepancies appearing at a few MeV. Nonuniqueness is also found in the NPA. The spread of energies used for $[L/M]_{n2}$ yields improved convergence at higher energies relative to $[L/M]_{n1}$. However, the smaller energy spread of $[L/M]_{n1}$ gives a better fit at low energies than does $[L/M]_{n2}$.

The NPA $[5/4]_{n1}$ has a simple pole and a simple zero which are nearly superimposed at $x \approx -1.090\,53$ fm⁻². This is not a defect because the point is in a region that is not physically accessible to elastic scattering. Such structure, seen in numerous examples in this investigation, is typical of the

manner in which Padé approximants sometimes represent branch points.[8] In this instance, comparison with $[5/4]_{n2}$, which has no such structure, but which is clearly superior at high energies to $[5/4]_{n1}$ (see Table IV), suggests that this structure is an artifact of the energy set used.

C. Hard core square well

Inasmuch as the hard core radius R can vary with the radial shape of potentials fitted to data, it is desirable to study more than one value of R. Two parametrizations, both fitting the experimental a_s and r_{0s}, are considered here. Potential A has $R = 0.5$ fm, leading to a momentum $k_c = 1.237\,870\,4$ fm⁻¹ at which the phase shift changes sign. Potential B has $R = 0.15$ fm. Such a small core radius is required with this radial shape if the change of sign of $\delta_0(k)$ is to occur in the experimental region. Here $k_c = 1.676\,53$ fm⁻¹ is in reasonable agreement with experiment.[6]

The potential parameters are b, which is the well radius as measured from the edge of the hard core, and V_0:

Potential A: $2\mu V_0 = 0.887\,691\,61$ fm⁻² ,

$$b = 1.623\,637\,4 \text{ fm} ,$$

Potential B: $2\mu V_0 = 0.419\,325\,38$ fm⁻² ,

$$b = 2.334\,836\,5 \text{ fm} .$$

Tables V and VI give values of $F(x)$ for potentials A and B, respectively. Two new classes of approximations introduced here are defined in terms of the hard core Padé transformation given in Sec. III C. $[L/M]_{tt}$ is obtained by finding the $[L/M]$ Padé approximant of the outer well, transforming it according to Eq. (3.7), and truncating the $[L/M]$; $[L/M]_{pt}$, shown here only for $[2/1]$, is the Padé approximant to $[L/M]_{tt}$, computed in each case by carrying all the hard core terms up to

TABLE III. Square well potential Padé coefficients.

Approximation	a_0 (fm⁻¹)	a_1 (fm⁻³)	a_2 (fm⁻⁵)	a_3 (fm⁻⁷)	a_4 (fm⁻⁹)	a_6 (fm⁻¹¹)	b_1 (fm⁻²)	b_2 (fm⁻⁴)	b_3 (fm⁻⁶)	b_4 (fm⁻⁸)
$[4/3]_t$	0.04216	1.385	0.7238	−2.788	4.702		0.1294	−2.398	4.611	
$[2/1]$	0.04216	1.364	0.1292				−0.3747			
$[2/1]_{n1}$	0.04256	1.365	0.1580				−0.3547			
$[2/1]_{n2}$	0.04259	1.362	0.3252				−0.2602			
$[3/2]_{n1}$	0.04216	1.350	−0.3315	0.06820			−0.7149	0.2087		
$[3/2]_{n2}$	0.04216	1.352	−0.2655	0.08421			−0.6662	0.1958		
$[4/3]_{n1}$	0.04216	1.345	−0.4955	0.1455	−0.003125		−0.8372	0.3231	−0.03446	
$[4/3]_{n2}$	0.04216	1.345	−0.4800	0.1423	−0.002174		−0.8257	0.3153	−0.03218	
$[5/4]_{n1}$	0.04216	1.384	0.7427	−0.3054	0.1300	0.002601	0.08346	−0.4438	0.2602	−0.03092
$[5/4]_{n2}$	0.04216	1.339	−0.6758	0.2162	−0.02363	0.001641	−0.09714	0.4385	−0.08000	0.005261

TABLE IV. Values of scattering function $F(x)$ for square well potential at various energies.

Approximation	1 MeV	10 MeV	$F(x)$ (fm^{-1}) 30 MeV	50 MeV	100 MeV	200 MeV
Exact	0.075 82	0.4160	1.471	2.980	6.167	10.79
$[4/3]_t$	0.075 82	0.4131	1.045	1.359	2.451	4.869
$[3/2]_t$	0.075 82	0.4252	−2.284	0.9112	2.495	5.342
$[2/1]$	0.075 82	0.4162	1.504	3.419	42.32	−11.93
$[2/1]_{n1}$	0.075 82	0.4161	1.496	3.350	4.822	−20.79
$[2/1]_{n2}$	0.076 10	0.4160	1.476	3.143	4.320	14.00
$[3/2]_{n1}$	0.075 82	0.4160	1.471	2.961	4.749	2.697
$[3/2]_{n2}$	0.075 81	0.4160	1.471	2.978	5.521	4.198
$[4/3]_{n1}$	0.075 82	0.4160	1.471	2.980	6.210	15.77
$[4/3]_{n2}$	0.075 82	0.4160	1.471	2.980	6.179	13.68
$[5/4]_{n1}$	0.075 82	0.4160	1.471	2.980	6.198	14.98
$[5/4]_{n2}$	0.075 82	0.4160	1.471	2.980	6.167	10.13

$[4/3]$ before finding the first four terms of the effective range expansion, from which a $[2/1]$ Padé is obtained exactly.

Defective approximants occur frequently here. The narrow singularities in $F(x)$ thereby created may even be hard to detect in a coarse scan of energies. In all cases presented in this paper the zeros of defective PA and NPA do not occur at low positive energies, preserving some usefulness for interpolation and determining effective range parameters. Increasing the spread of energies fitted with the NPA algorithm simultaneously increases the region of validity of the fit and decreases the chance of there being a defect.

The general trend in Tables V and VI is clear: Padé approximants are superior to truncation; higher orders of PA and NPA are better at higher energies than low orders, provided they are not defective; $F(x)$ is better approximated by low-order PA in the case of potential A, where the pole is at a lower value of x than in the case of potential B. Clearly, care must be taken to scrutinize the NPA because those containing defective behavior must not be considered as legitimate analytic continuations of the effective range expansions. The hard core Padé transformation is most effective when used to generate a series from which a PA is obtained. This is seen in the

TABLE V. Values of scattering function $F(x)$ for hard core square well potential, potential A, with $R = 0.5$ fm, at various energies.

Approximation	1 MeV	10 MeV	50 MeV	100 MeV	200 MeV
	0.075 90	0.4292	7.083	−4.666	−2.026
$[2/1]$	0.075 90	0.4292	7.111	−4.552	−1.791
$[2/1]_{n1}$	0.075 90	0.4292	7.109	−4.554	−1.792
$[2/1]_{n2}$	0.075 90	0.4292	7.098	−4.570	−1.803
$[3/2]_{n1}$	0.075 90	0.4292	7.165	−4.536	−1.785
$[3/2]_{n2}$	0.075 90	0.4292	7.082	−4.867	−1.724
$[4/3]_{n1}$	0.075 90	0.4292	7.082	−4.667	−2.051
$[4/3]_{n2}$	0.075 90	0.4292	7.083	−4.667	−2.038
$[3/2]_t$	0.075 90	0.4304	−10.440	0.3799	2.918
$[4/3]_t$	0.075 90	0.4290	3.833	3.270	3.741
$[4/3]_{tt}$	0.075 90	0.4292	7.051	−4.816	−2.392
$[2/1]_{pt}$	0.075 90	0.4292	7.111	−4.552	−1.791
$[3/2]_{tt}$	0.075 90	0.4292	6.846	−5.229	−2.669
$[2/1]_{pt}$	0.075 90	0.4292	7.112	−4.551	−1.791
$[2/1]_{tt}$	0.075 90	0.4275	5.128	−10.3200	−4.253
$[2/1]_{pt}$ [a]	0.075 91	0.4292	7.050	−4.633	−1.843

[a] The $[2/1]_{pt}$ are computed using the series generated by the $[L/M]_{tt}$ immediately above each entry.

TABLE VI. Values of scattering function $F(x)$ for hard core square well potential, potential B, with $R=0.15$ fm, at various energies.

Approximation	1 MeV	10 MeV	$F(x)$ (fm^{-1}) 50 MeV	100 MeV	200 MeV	300 MeV
Exact	0.075 85	0.4213	3.960	52.36	−24.03	−11.55
$[2/1]$	0.075 85	0.4214	4.307	−15.66	−4.734	−3.879
$[2/1]_{n1}$	0.075 85	0.4213	4.250	−17.41	−5.036	−4.178
$[2/1]_{n2}$	0.075 95	0.4213	4.082	−29.47	−6.577	−5.707
$[3/2]_{n1}$	0.075 85	0.4213	3.947	23.58	4.337	2.640
$[3/2]_{n2}$	0.075 85	0.4213	3.958	35.62	10.16	5.573
$[4/3]_{n1}$	0.075 90	0.4213	3.960	52.51	−21.21	−8.412
$[4/3]_{n2}$	0.075 85	0.4213	3.960	52.46	−21.51	−8.542
$[4/3]_{n2}$	0.075 85	0.4213	3.960	52.46	−21.51	−8.542
$[5/4]_{n1}$	0.075 85	0.4213	3.960	52.57	−21.07	−8.364
$[5/4]_{n2}$	0.075 85	0.4213	3.960	52.35	35.50	−7.529
$[6/5]_{n1}$ [a]	0.075 85	0.4213	3.960	52.58	−21.04	−8.354
$[6/5]_{n2}$ [a]	0.075 85	0.4213	3.960	52.36	−24.04	−11.62
$[4/3]_{tt}$	0.075 85	0.4213	3.962	56.09	−18.53	−7.504
$[2/1]_{pt}$	0.075 85	0.4214	−476.8	−0.7572	1.187	2.584
$[2/1]_{tt}$	0.075 96	0.4205	3.746	251.5	−10.51	−9.169
$[2/1]_{pt}$	0.075 96	0.4213	4.062	−31.90	−6.782	−5.904

[a] Defective approximants containing zeros in P and Q at nearly equal positive energies.

last six entries of Tables V and VI.

One other test is the ability of these approximations to locate the singularity. As shown in Table VII, results similar to these of Tables V and VI obtain. The failure of $[3/2]_n$ to produce a pole in the right region for potential B highlights the uncertainty in the rate at which convergence sets in, particularly when the pole is so distant from the origin.

TABLE VII. Location of singularities in $F(x)$ for various approximations, for HCSW potentials A and B.

Method	Potential A $E_{\text{c.m.}}$ (MeV)	Potential B $E_{\text{c.m.}}$ (MeV)
Exact	63.55	116.47
$[4/3]_t$	a	a
$[3/2]_t$	46.37[b]	32.37[b]
$[2/1]$	63.41	82.33
$[2/1]_{n1}$	63.41	83.56
$[2/1]_{n2}$	63.45	88.77
$[3/2]_{n1}$	63.33[c]	a
$[3/2]_{n2}$	63.57[d]	a
$[4/3]_{n1}$	63.55	116.35
$[4/3]_{n2}$	63.55	116.42
$[5/4]_{n1}$	63.55[c]	116.29[c]
$[5/4]_{n2}$	63.55	116.60
$[6/5]_{n1}$	63.55[c]	116.33[c]
$[6/5]_{n2}$	63.55[c]	116.57[c]

[a] No singularity under 300 MeV.
[b] Oscillations of sign occur at low energies.
[c] These are defective.
[d] These oscillate (see Tables V and VI).

It is not necessary to assume that the singularity in $F(x)$ is a pole if the phase shifts are known numerically with precision. Another Padé technique, the d/dx logarithm method,[8] gives the power γ of the singularity in $F(x)$ when evaluated at points near x_0, where $F(x) \sim (x - x_0)^{-\gamma}$. A crude scan of $(x - x_0)(d/dx)\ln[F(x)]$ through the singular point has been carried out and has yielded $\gamma = 1 \pm 0.000\,04$ for potential A and $\gamma = 1 \pm 0.001$ for potential B. Here departure from $\gamma = 1$ is principally a measure of the errors of the numerical scanning procedure and the location of the pole. More complete use of the power of Padé techniques can be utilized to determine both x_0 and γ more accurately if needed.[8]

D. Hard core Yukawa

As a final application we present results for a physically more realistic potential,[3] for which analytic scattering solutions are not known:

$$V(r) = \infty, \quad r < R$$

$$V(r) = -V_0 \frac{\exp(-r/b)}{(r/b)}, \quad r \geq R$$

with parameters $R = 0.4$ fm, $b = 0.7$ fm, and $V_0 = 415.8896$ MeV, where we have made adjustments of the parameters given by Brown and Jackson[3] to conform to the physical constants adopted in this paper. The phase shift changes sign at $E_{\text{c.m.}} = 113.562$ MeV, which is reasonable. As the effective range expansion is not known, strictly numerical methods must be used throughout. We have

TABLE VIII. Low energy values of $F(x)$ for HCY potential.

Method	1 MeV	2 MeV	$F(x)$ (fm^{-1}) 3 MeV	4 MeV	5 MeV	10 MeV
Exact	0.075 669 9	0.109 601	0.143 971	0.178 800	0.214 109	0.398 548
$[2/1]_{n3}$	0.075 669 8	0.109 601	0.143 971	0.178 800	0.214 108	0.398 622
$[2/1]_{n4}$	0.075 852 7	0.109 707	0.144 024	0.178 820	0.214 109	0.398 548
$[2/1]_{n5}$	0.075 545 3	0.109 350	0.143 634	0.178 411	0.213 695	0.398 287
$[3/2]_{n3}$[a]	0.075 669 8	0.109 601	0.143 971	0.178 800	0.214 109	0.398 640
$[3/2]_{n4}$	0.075 630 9	0.109 579	0.143 960	0.178 791	0.241 109	0.398 548
$[3/2]_{n5}$	0.075 661 6	0.109 585	0.143 951	0.178 779	0.214 088	0.398 539
$[4/3]_{n3}$[a]	0.075 669 9	0.109 601	0.143 971	0.178 800	0.214 109	0.398 548
$[4/3]_{n4}$[a]	0.075 680 2	0.109 606	0.143 973	0.178 801	0.214 109	0.398 548
$[3/2]_{c6}$	0.075 672 5	0.109 601	0.143 961	0.178 776	0.214 067	0.398 440
$[3/2]_{c7}$	0.075 659 3	0.109 653	0.144 058	0.178 901	0.214 204	0.398 453
$[3/2]_{c8}$	0.075 670 6	0.109 599	0.143 965	0.178 789	0.214 092	0.249 897

[a] These NPA have defects which appear at energies well above the energy region shown here.

numerically integrated the Schrödinger equation using the Noumerov method,[20] with an estimated fractional error in the phase shifts close to 10^{-9}, thereby generating high quality data. It is of interest here that defects occur earlier in the Padé table, i.e., for lower values of L, than in any of the previous examples. Clearly, if a precision of 10^{-9} generates defective NPA, then there are potential difficulties in using the method on experimental data. Therefore, we have chosen this example for testing χ^2 minimization and least-squares fitting procedures as some important alternatives.

It is important to scrutinize the low-energy fits of the various approximations to help judge which set of effective range parameters is most correct. Table VIII compares various NPA values of $F(x)$ from 1 to 10 MeV. The two best approximants, $[4/2]_{n3}$ and $[3/2]_{n3}$, are both defective at

energies far displaced from the range ($E_{c.m.} \leq 10$ MeV) shown. However, the effective range parameters obtained in this example by expanding the various NPA functions are likely to be best described in terms of these two approximants. Values of a, r_0, P, and Q are given in Table IX for most of the cases of interest, including χ^2 minimization and a least-squares fit. Table X compares values of $F(x)$ at higher energies and gives the location of the singularity in terms of the energy E_c at which the phase shift changes sign.

Among the NPA shown in the tables, $[3/2]_{n5}$ appears to be optimal over the entire range shown. We have been unable to find an energy set for which we can obtain a $[4/3]_n$ which is not defective and which at the same time gives a good fit at all energies.

The χ^2-minimized approximants, namely $[3/2]_{c6}$ and $[3/2]_{c8}$, give values of effective range param-

TABLE IX. Effective range parameters for HCY potential for various approximations including χ^2 minimization and least squares; location of singularity at E_c and radius of convergence at E_p.

Method	a (fm)	r_0 (fm)	P	Q	χ^2	E_c (MeV)	E_p (MeV)
Exact						113.56	
$[3/2]_{n3}$	−23.719	2.7624	−0.016 484	0.001 234 25		a	
$[3/2]_{n4}$	−23.757	2.7653	−0.015 745	0.001 767 5		107.95	
$[3/2]_{n5}$	−23.718	2.7615	−0.016 532	0.001 405 5		113.56	
$[4/3]_{n3}$	−23.720	2.7627	−0.016 267	0.001 525 9		a	
$[3/2]_{c6}$	−23.724	2.7640	−0.015 619 9	0.001 857 70	0.013 37	113.76	27.19
$[3/2]_{c7}$	−23.780	2.7722	−0.014 495 8	0.002 037 11	56.288[b]	113.57	27.23
$[3/2]_{c8}$	−23.720	2.7633	−0.015 903 7	0.001 795 46	0.001 29	113.06	24.93

[a] These are defective NPA and are therefore considered to be unreliable for locating E_c and E_p.

[b] This χ^2 is a least-squares value multiplied by 10^4 and is therefore comparable with the other examples given.

TABLE X. Values of $F(x)$ for HCY potential, including location of singularity (E_c).

Method	$F(x)$ (fm^{-1}) 100 MeV	200 MeV	300 MeV	E_c (MeV)
Exact	23.9177	−6.61065	−4.02834	113.562
$[2/1]_{n3}$	0.00357438	−3.04790	5.27639	62.7783
$[2/1]_{n4}$	−2.07523	2.06248	4.19076	72.943
$[2/1]_{n5}$	39.1442	−3.70196	−1.27924	106.753
$[3/2]_{n4}$	35.381	−4.57273	−2.21655	107.954
$[3/2]_{n5}$	23.9152	−6.60657	−4.03336	113.563

eters that are close to the best ones, while coming realistically close to the true value of E_c. Restricting the χ^2 minimization to lower energies ($E_{c.m.} < 70$ MeV for $[3/2]_{c8}$) appears to lead to excellent effective range parameters while coming close to E_c as well. The least-squares fit, namely $[3/2]_{c7}$, gives an excellent value of E_c while producing only slightly inferior values of the effective range parameters. The d/dx logarithm method, when applied to the numerical phase shifts, leads to a value of 1 ± 0.00009 of the power γ of the singularity, establishing the existence of a simple pole.

With such a low χ^2 (0.01337) and such close numerical agreement in general, it is tempting to conclude that our minimization procedures using MINIRAT are a practical means of performing an analytic continuation. However, we cannot absolutely rule out other good χ^2 values in other regions of Padé parameter space. In the light of this uncertainty another numerical experiment has been performed. As we discuss more fully in the concluding section, the sign of a_4 in $P_3(x)$ is crucial in the solution of the inverse scattering problem.[13] Where χ^2 minimization has been performed on the experimental phase shifts, a_4 is found to be positive, leading to a solvable inverse scattering problem.[9,14] Invariably a_4 is negative in all our $[3/2]$ fits to the HCY potential problem, yielding an unsolvable inverse scattering problem. We have chosen Padé parameters that are characteristic of the fits to the MAW phase shifts, with $a_4 > 0$, for the starting point of our χ^2-minimization routine. The approximant in Table IX, with $a_4 < 0$ and $\chi^2 = 0.00129$, is the end result after 90 iterations from that starting point. The imprint of the hard core, then, seems unmistakable in this example.

V. DISCUSSION

NPA techniques provide a basis for an accurate description of the s-wave scattering function for a variety of central potentials. To illustrate the NPA we have chosen examples with features characteristic of the np $^1S_0$ state. The presence of a hard core, often introduced in describing this state, creates both a simplification and a complication. The simplification derives from the ease of accurate description of $F(x)$ when it has a simple pole singularity. Such a structure, particularly appropriate for Padé methods, in our examples leads to good fits using $[3/2]$ approximants.

The complication with the hard core lies in the impossibility in all our examples of solving the inverse scattering problem using the Marchenko method. We have checked every example which contains a hard core, and we have found that the condition $\delta(0) - \delta(\infty) = 0$ is never satisfied, just as it is not satisfied for the hard core alone. Although the Marchenko method is not of use as it stands, a modification of it using the hard core Padé transformation should be possible. We will sketch the proposed procedure, the practicality of which is currently under investigation. We suppose we are given an NPA of a scattering function $F(x)$ for which $\delta(0) - \delta(\infty) \neq 0$ but which does not support a bound state. Assuming a value for a hard core radius, we use Eqs. (3.7) and (3.8) to find the Taylor series for the scattering function of the external potential. We then obtain the PA and, if possible, solve the Marchenko equations for the potential, iterating the hard core radius if needed. Although it is clearly possible in this way to retrieve a potential containing a hard core, there are some unresolved questions of uniqueness.

Interestingly, the phase shifts of MAW derived from experiment lead directly to solutions of the Marchenko equations.[9,14] This may be construed as indirect evidence, although hardly conclusive, that an infinite hard core does not occur in the np $^1S_0$ state. The contrasting behavior of the scattering function for the HCY potential and for fits to the $^1S_0$ np phase shifts of MAW is shown in Fig. 1.

Two other results should be stressed. First, the χ^2-minimization approach to the NPA is an efficient technique for approximating the scattering function, locating poles and also achieving an approximate analytic continuation. Consider the HCY example. For $[3/2]_{c8}$, the low energy values at $E_{c.m.} \leq 70$ MeV are used to obtain values of $F(x)$ at intermediate energies for $E_{c.m.} \lesssim 300$ MeV. In this example, the radius of convergence of the Taylor series for $[3/2]_{c8}$ is 24.93 MeV. This result, shown in the last column of Table IX, is obtained simply by factoring the denominator polynomial. That data which are at energies beyond the radius of convergence may be used for analytic continuation serves to illustrate the flexibility of
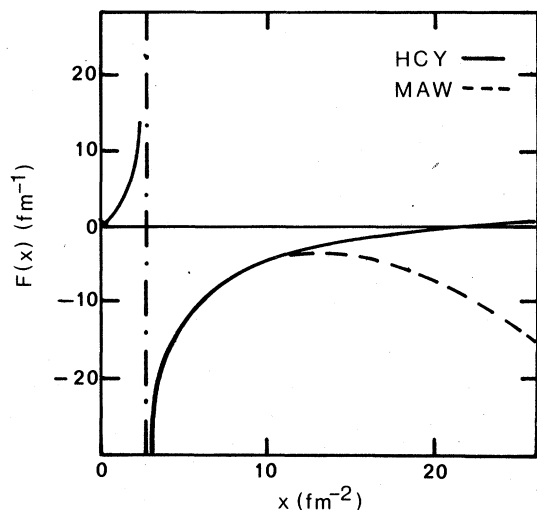
FIG. 1. Contrasting behavior of scattering function $F(x) = k \cot(\delta_0)$ for HCY potential (———) and fits to $^1S_0$ np phase shifts of MAW (Ref. 6) (-----). For an example of such a fit, see Ref. 14.

this method.

Finally, not only do χ^2 minimization and least-squares NPA locate poles with high precision, but they are also seen to provide accurate interpolation by a method which simulates the analysis of real experimental data. This is shown for the

HCY example in Tables VIII, IX, and X. In Table VIII the values of F shown represent excellent interpolations for the energy sets $n3$, $n4$, and $n5$, while the values for the χ^2-minimized sets, $C6$, $C7$, and $C8$ are also close. This high accuracy is representative of the observed interpolations in all examples we have studied. Therefore, the HCY results suggest that such a small number of parameters as six can be useful in accurately describing central force scattering experiments over a wide energy range within the framework of a Padé ansatz, even if that ansatz does not lead to a solution of the inverse scattering problem. It remains to be seen whether a similar economy of description is possible for the considerably more complicated triplet np state.

[1]*Nucleon-Nucleon Interactions*, Proceedings of the Second International Conference on Nucleon-Nucleon Interactions, Vancouver, 1977, edited by D. F. Measday, H. W. Fearing, and A. Strathdee (AIP, New York, 1978), referred to hereinafter as MFS, gives a detailed account of the status of this problem.

[2]R. Vinh Mau, in Ref. 1, p. 140.

[3]A. D. Jackson, D. O. Riska, and B. Verwest, Nucl. Phys. A249, 397 (1975); also see G. E. Brown and A. D. Jackson, *The Nucleon-Nucleon Interaction* (North-Holland/American Elsevier, New York, 1976), referred to hereinafter as BJ.

[4]M. Lacombe *et al.*, Phys. Rev. D 12, 1495 (1975).

[5]D. W. L. Sprung, in Ref. 1, p. 209, reviews a decade of work in developing and using SSC models.

[6]M. H. MacGregor, R. A. Arndt, and R. M. Wright, Phys. Rev. 182, 1714 (1969), hereinafter referred to as MAW, and preceding papers cited therein. MAW obtained phase shifts that have been heavily relied upon by developers of potential models.

[7]M. K. Srivastava and D. W. L. Sprung, in *Advances in Nuclear Physics* (Plenum, New York, 1975), Vol. 8, p. 121, review the phenomenology of adducing the off-shell *NN* interaction.

[8]G. A. Baker, Jr., *Essentials of Padé Approximants* (Academic, New York, 1975), is a comprehensive review which discusses physical applications and pro-

vides the notation used in this paper. Except where otherwise indicated, Baker refers to this monograph.

[9]K. Hartt (unpublished).

[10]E. Lomon and R. Wilson, Phys. Rev. C 9, 1329 (1974).

[11]R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).

[12]V. de Alfaro and T. Regge, *Potential Scattering* (American Elsevier, New York, 1965).

[13]F. Lambert, O. Corbella, and Z. D. Thomé, Nucl. Phys. B90, 267 (1975), referred to hereinafter as LCT.

[14]D. W. L. Sprung and M. K. Srivastava, Nucl. Phys. A139, 605 (1969).

[15]G. A. Viano, Nuovo Cimento 63A, 581 (1969).

[16]K. Hartt (unpublished).

[17]R. W. Haymaker and L. Schlessinger, in *The Padé Approximant in Theoretical Physics*, edited by G. A. Baker, Jr. and J. L. Gammel (Academic, New York, 1970), pp. 257–287 and references cited therein. Referred to in the present paper as HS.

[18]K. Hartt, Bull. Am. Phys. Soc. 22, 117 (1977); 23, 630 (1978).

[19]E. R. Cohen and B. N. Taylor, J. Phys. Chem. Ref. Data 2, 663 (1973).

[20]M. A. Melkanoff, T. Sawada, and J. Raynal, in *Methods in Computational Physics*, edited by B. Adler, S. Fernbach, and M. Rotenberg (Academic, New York, 1966), Vol. 6, pp. 1–80.