PADÉ APPROXIMATION IN EFFECTIVE RANGE THEORY

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Padé approximation has been proposed for calculating the scattering length and the effective range as functions of the potential strength. The appropriate Taylor series coefficients which constitute input for the Padé method are obtained from a perturbative scheme based on the variable phase method.

1. Introduction

The purpose of this paper is to show that the Padé approximation combined with the variable phase method results in a very effective scheme for evaluating the s-wave scattering length a and the effective range r_0. According to the standard methods, given the potential, these parameters may be obtained after a single integration of the appropriate s-wave Schrödinger equation and if we want a and r_0 for several values of the potential strength the integration procedure has to be applied repeatedly. The advantage of the proposed method lies in the fact that after a single integration one is given the functional dependence of a and r_0 upon the strength of the potential. Thus, in contrast with the standard methods which produce just two numbers, the proposed method gives two functions after the same amount of labour.

The plan of the presentation is as follows. In Section 2 we discuss the analytic properties of a and r_0 regarded as functions of the potential strength and give a brief account of the necessary essentials of the Padé approximation. In Section 3 we develop a perturbative expansion scheme based on the variable phase method which gives the appropriate Taylor expansion coefficients to be used as input for constructing the Padé approximants. In Section 4 we illustrate the effectiveness of the proposed scheme in the case of the Hulthén potential and in Section 5 we discuss the conditions for the existence of a bound state in a given potential. Finally, in Section 6 we present our conclusions.

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2. Padé approximation

We shall consider s-wave scattering of a particle of mass μ by a local central potential $V(r)$. We assume that the potential is less singular at $r = 0$ than r^{-2} and is of a short range which means that it has a sufficiently rapid fall-off so that both a and r_0 should exist: If the potential does not change sign, what will be assumed in the following, a convenient measure of the strength is given by the dimensionless quantity s, defined as

$$s = -2\mu \int_0^\infty V(r) r dr \tag{1}$$

($h = c = 1$ units adopted hereafter). The scattering length and the effective range may be both thought as functions of s and the usual effective range expansion takes the form which exhibits the dependence on s

$$k \cot \delta(k, s) = -[a(s)]^{-1} + \tfrac{1}{2} k^2 r_0(s) + O(k^4), \tag{2}$$

where k is the wave number and $\delta(k, s)$ is the s-wave phase shift.

Elsewhere [1] we have shown that $a(s)$ and $r_0(s)$ are meromorfic functions of s and may be represented as quotients of two entire functions, viz.

$$a(s) = P(s)/Q(s), \tag{3}$$

$$r_0(s) = R(s)/[P(s)]^2, \tag{4}$$

where the functions $P(s)$, $Q(s)$ and $R(s)$ may be conveniently represented in a product form (cf. Ref. [1])

$$P(s) = a_1 s \prod_{n=1}^{\infty} (1 - s/z_n), \tag{5a}$$

$$Q(s) = \prod_{n=1}^{\infty} (1 - s/s_n), \tag{5b}$$

$$R(s) = 2\beta_1 s(1 - \xi_0 s) \prod_{n=1}^{\infty} (1 + \xi_n s + \eta_n s^2). \tag{5c}$$

The constants a_1, z_n, s_n, β_1, ξ_n, and η_n are real and depend upon the shape of the potential. In particular, a_1 and β_1 are given by the expressions [1]

$$a_1 = -\frac{\int_0^\infty V(r) r^2 dr}{\int_0^\infty V(r) r dr}, \qquad \beta_1 = \tfrac{1}{3} \frac{\int_0^\infty V(r) r^4 dr}{\int_0^\infty V(r) r dr}. \tag{6}$$

In practical applications $P(s)$, $Q(s)$, and $R(s)$ may be approximated with arbitrary accuracy by polynomials and usually just a few factors in (5) turns out to be sufficient. This comes about because the potentials we have to deal with considering strongly interacting systems such as NN, $\overline{\text{K}}$N, ΛN, etc. may support at most one bound state. Therefore, what we are interested in is in fact the behaviour of $P(s)$, $Q(s)$ and $R(s)$ in a limited range of s values $-3.0 \leqslant s \leqslant 3.0$.

The representation of $a(s)$ and $r_0(s)$ as a ratio of two polynomials suggests that they should be obtainable in result of the application of the Padé approximation. Since the latter method has been described in many places, we shall confine our attention to a review of the necessary essentials (a current review of the subject may be found in Refs. [2] and [3]).

Let us consider then a function $f(s)$ which vanishes at $s = 0$ and is analytic in the neighbourhood of zero. The Taylor series

$$f(s) = \sum_{n=1}^{\infty} f_n s^n \tag{7}$$

converges within a circle around $s = 0$ which passes through the nearest singularity. Although the Taylor series (7) cannot be used to evaluate $f(s)$ outside the circle of convergence but, of course, the function $f(s)$ is uniquely determined by the coefficients f_n. The Padé method makes use of these coefficients to obtain an approximate analytic continuation of $f(s)$ beyond the convergence circle of (7). We shall be concerned here with the so called diagonal Padé approximation, where $f(s)$ is being sought as a ratio of two polynomials both of the order N ($N = 1, 2, 3, \ldots$), viz.

$$f(s) \simeq f^{[N,N]}(s) \equiv \frac{P^{[N]}(s)}{Q^{[N]}(s)}, \tag{8}$$

where

$$P^{[N]}(s) = \sum_{n=1}^{N} p_n s^n, \tag{9}$$

$$Q^{[N]}(s) = \sum_{n=0}^{N} q_n s^n, \tag{10}$$

and the hitherto unknown coefficients p_n and q_n are determined by the requirement that the lowest $2N$ derivatives of $f(s)$ and those of the $f^{[N,N]}$ approximant should coincide at $s = 0$. This condition gives $(2N+1)$ linear equations whose explicit solution is

$$p_n = \begin{vmatrix} f_1 f_2 & \cdots & f_{N+2-n} & \cdots & f_{N+1} \\ f_2 f_3 & \cdots & f_{N+3-n} & \cdots & f_{N+2} \\ \vdots\ \vdots & & \vdots & & \vdots \\ f_N f_{N+1} & \cdots & f_{2N+1-n} & \cdots & f_{2N} \\ 0\ 0 & \cdots & f_1 & \cdots & f_n \end{vmatrix}, \tag{11}$$

$$q_n = \begin{vmatrix} f_1 f_2 & \cdots & f_{N+1-n} & \cdots & f_{N+1} \\ f_2 f_3 & \cdots & f_{N+2-n} & \cdots & f_{N+2} \\ \vdots\ \vdots & & \vdots & & \vdots \\ f_N f_{N+1} & \cdots & f_{2N-n} & \cdots & f_{2N} \\ 0\ 0 & \cdots & 1 & \cdots & 0 \end{vmatrix}. \tag{12}$$

The advantage of the Padé method lies in the fact that knowing the behaviour of $f(s)$ close to zero, one may find approximately the singularities of $f(s)$ by looking for the zeros of $Q^{[N]}(s)$.

Having assembled all the necessary tools, we can return now to $a(s)$ and $r_0(s)$, but before we start applying the Padé method we have to dispose of a minor difficulty. Inspection of the expression (3)—(5) indicates that only $a(s)$ vanishes at $s = 0$ whereas $r_0(s)$ has a pole at $s = 0$. The simplest way out is to introduce an entire function $\beta(s)$ which vanishes at $s = 0$ and seek $r_0(s)$ in the form

$$r_0(s) = \frac{2\beta(s)}{[a(s)]^2} . \tag{13}$$

The factor 2 is introduced for a later convenience and by construction $r_0(s)$ has the correct $1/s$ behaviour for s values close to zero. Our task is now to devise an effective scheme for evaluating the appropriate Taylor series coefficients for $a(s)$ and $\beta(s)$ expanded around $s = 0$ to be used as input in the expressions (8) — (12). This will be accomplished in the following section by using the variable phase method.

3. Variable phase perturbative scheme

The variable phase method has been described in many places (a rather complete review may be found in Ref. [4]). Basically, the chief idea behind this method is to eliminate the usual radial wave function in favour of the variable phase $\Delta(r)$ so that the Schrödinger equation can be rewritten as a differential equation for $\Delta(r)$. The corresponding phase shift $\delta(s, k)$ is obtained as the limit of $\Delta(r)$ for $r \to \infty$. For low energies one may expand $\Delta(r)$ in powers of k, viz.

$$(-1/k) \tan \Delta(r) = A(r) + B(r)k^2 + O(k^4), \tag{14}$$

where $A(r)$ and $B(r)$ are two functions to be determined and in (14) the dependence on s has been suppressed. Clearly, for $r \to \infty$ formula (14) goes over into the usual effective range expansion (2), and we find

$$a = \lim_{r \to \infty} \Delta(r), \tag{15}$$

$$\beta = \lim_{r \to \infty} B(r). \tag{16}$$

Using the Schrödinger equation for $\Delta(r)$, it can be shown [4] that $A(r)$ and $B(r)$ are solutions of the following differential equations

$$A'(r) = -sU(r)\,[r - A(r)]^2, \tag{17}$$

$$B'(r) = sU(r)\,\{\tfrac{1}{3}r^4 + r[B(r) - \tfrac{4}{3}r^2 A(r)] + [A(r)r^2 - B(r)]\,A(r)\} \tag{18}$$

where the potential $U(r)$ is defined as

$$U(r) = V(r)\left[\int_0^\infty V(x)xdx\right]^{-1} \tag{19}$$

and does not depend on s. The boundary conditions are $A(0) = B(0) = 0$.

For small s we can represent $A(r)$ and $B(r)$ in a power series form, viz.

$$A(r) = \sum_{n=1}^{\infty} A_n(r)s^n, \tag{20}$$

$$B(r) = \sum_{n=1}^{\infty} B_n(r)s^n. \tag{21}$$

Setting $r \to \infty$ in (20) and (21), we obtain the desired Taylor expansions for $a(s)$ and $\beta(s)$, respectively

$$a(s) = \sum_{n=1}^{\infty} a_n s^n, \tag{22}$$

$$\beta(s) = \sum_{n=1}^{\infty} \beta_n s^n, \tag{23}$$

where

$$a_n = \lim_{r\to\infty} A_n(r), \quad \beta_n = \lim_{r\to\infty} B_n(r). \tag{24}$$

Inserting the expansions (20) and (21) in (17) and (18), and equating the coefficients multiplying the different powers of s, we obtain an infinite system of equations for the $A_n(r)$ and $B_n(r)$ functions. These equations are trivially solved by quadrature and we end up with the recurrences

$$A_1(r) = -\int_0^r U(x)x^2dx, \quad A_2(r) = 2\int_0^r U(x)xA_1(x)dx,$$

$$A_{n+2}(r) = \int_0^r U(x)\left[2xA_{n+1}(x) - \sum_{j=0}^{n-1} A_{j+1}(x)A_{n-j}(x)\right]dx, \tag{25}$$

$$B_1(r) = \tfrac{1}{3}\int_0^r U(x)x^4dx, \quad B_2(r) = \int_0^r U(x)x\left[B_1(x) - \tfrac{4}{3}x^2A_1(x)\right]dx,$$

$$B_{n+2}(r) = \int_0^r U(x)\left\{x\left[B_{n+1}(x) - \tfrac{4}{3}x^2A_{n+1}(x)\right]\right.$$

$$\left. + \sum_{j=0}^{n-1} A_{j+1}(x)\left[x^2A_{n-j}(x) - B_{n-j}(x)\right]\right\}dx, \quad n = 1, 2, 3 \cdots. \tag{26}$$

The resulting system of equations (25) and (26) is very simple and for many potential shapes the $A_n(r)$ and $B_n(r)$ functions may be obtained in an analytic form. The recurrences (25) and (26) complete our scheme and letting $r \to \infty$ from (24) we immediately obtain the a_n and β_n coefficients necessary for constructing the Padé approximants.

Some care has to be exercised, however, in setting the order N of the Padé approximants. As far as $a(s)$ is concerned, N is of course arbitrary, and increasing N we account for additional poles and zeros extending thereby the accuracy and the range of applicability of the Padé approximant. This is not quite that simple in the case of $\beta(r)$. Since the only poles of $r_0(s)$ appear at the zeros of $a(s)$, the poles that occur in $\beta(s)$ have got to be canceled with the poles in $[a(s)]^2$. As seen from formula (13), the Padé approximants for $\beta(s)$ ought to be chosen in such a way as to obtain only second order poles which in the limit $N \to \infty$ would be exactly cancelled with the poles that occur in $[a(s)]^2$. Therefore, the Padé approximants to $\beta(s)$ have to be of the order $2N$, for then both the numerator and the denominator in (13) are approximated by polynomials of the same order. Summarizing, we suggest the following approximation scheme

$$a(s) \simeq a^{[N,N]}(s),$$

$$r_0(s) \simeq 2\beta^{[2N,2N]}(s)\,\{a^{[N,N]}(s)\}^{-2}.$$

Consequently, the coefficients a_n have to be evaluated up to $2N$ and, correspondingly, the coefficients β_n up to $4N$.

4. Numerical example

In this section we shall illustrate the effectiveness and accuracy of the method described in the preceding section by calculating $a(s)$ and $\beta(s)$ for the Hulthén potential of the form

$$V(r) = -V_0[\exp(r/R)-1]^{-1}, \tag{27}$$

where V_0 and R are the depth and range parameters, respectively. Since for Hulthén's potential exact expressions for $a(s)$ and $r_0(s)$ may be obtained (cf. Ref. [1]), we can readily examine the effectiveness and accuracy of the Padé approximants. In this case the coefficients a_n and β_n are given by the following expressions

$$a_n = -2R(6/\pi^2)^n\zeta(2n+1),$$

$$\beta_n = (4/3)R^3(6/\pi^2)^n(n+1)\,(n+2)\zeta(2n+3)+\tfrac{1}{3}\sum_{m=1}^{n-2}\sum_{j=1}^{n-m-1} a_m a_j a_{n-m-j},$$

where $\zeta(z)$ is Riemann zeta function and it is understood that $a_j = 0$ for $j < 1$. The strength parameter s is related to V_0 and R by the formula

$$s = (\pi^2/3)\,\mu V_0 R^2$$

and the $1s$, $2s$, $3s$, ... zero-energy bound states appear at s values equal $s_n = (\pi^2/6)n^2$ with $n = 1, 2, 3, \ldots$ In Table I we compare the Padé approximants for $N = 1, 2, 3, 4, 5$ with the exact values of $a(s)$ for s in the range $-10.0 \leqslant s \leqslant 10.0$, whereas in Table II we examine the accuracy of the Padé method for calculating $\beta(s)$ for the same values of s and N.

TABLE I

The Padé approximants $a^{[N, N]}$ in units of R for the Hulthén potential (27) for different values of the strength parameter s

s	$a^{[1, 1]}$	$a^{[2, 2]}$	$a^{[3, 3]}$	$a^{[4, 4]}$	$a^{[5, 5]}$	a (exact)
−10.0	2.3	2.92	2.985	2.98718	2.987227	2.987227
−8.0	2.2	2.73	2.770	2.77122	2.771240	2.771240
−6.0	2.1	2.47	2.4953	2.495677	2.495680	2.495680
−4.0	1.9	2.108	2.1152	2.115260	2.115260	2.115260
−2.0	1.4	1.5020	1.5028	1.502830	1.502830	1.502830
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.5	− 0.99	−1.0036	−1.0036	−1.003578	−1.003578	−1.003578
1.0	−3.07	−3.3767	−3.3785	−3.378456	−3.378456	−3.378456
1.5	−10.3	−20.84	−21.1444	−21.145234	−21.145235	−21.145233
2.0	59.9	10.89	10.6238	10.622435	10.622433	10.622434
2.5	11.7	5.14	4.9713	4.969794	4.969790	4.969790
3.0	7.6	3.47	3.2658	3.26292	3.262905	3.262905
3.5	6.1	2.5	2.251	2.24443	2.244387	2.244387
4.0	5.3	1.9	1.399	1.3839	1.383810	1.383810
5.0	4.5	0.67	−0.69	−0.800	−0.80205	−0.802062
6.0	4.1	−0.72	−6.70	−8.345	−8.3913	−8.391701
7.0	3.8	−2.8	35.9	18.58	18.2629	18.259232
8.0	3.7	−6.6	9.0	6.97	6.8796	6.878131
9.0	3.5	−17.1	6.0	4.66	4.565	4.562824
10.0	3.4	−231.5	4.7	3.4	3.277	3.272986

TABLE II

The Padé approximants $\beta^{[2N, 2N]}$ in units of R^3 for the Hulthén potential (27) for different values of the strength parameter s

s	$\beta^{[2, 2]}$	$\beta^{[4, 4]}$	$\beta^{[6, 6]}$	$\beta^{[8, 8]}$	$\beta^{[10, 10]}$	β (exact)
−10.0	1.9	5.69	5.7898	5.789826	5.789799	5.789846
−8.0	1.3	3.98	4.0261	4.026050	4.026042	4.026052
−6.0	0.5	2.145	2.1594	2.159443	2.159441	2.159441
−4.0	−5.0	0.2238	0.2261	0.226103	0.226100	0.226102
−2.0	−1.6	−1.5180	−1.5179	−1.517921	−1.517921	−1.517922
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.5	5.02	5.0084	5.0084	5.008353	5.008353	5.008353
1.0	31.3	28.970	28.9693	28.969299	28.969299	28.969300
1.5	−122.5	760.87	744.8289	744.828949	744.828948	744.829355
2.0	−52.7	142.9	132.4436	132.443652	132.443647	132.443719
2.5	−51.0	25.1	20.4247	20.424775	20.424763	20.424772
3.0	−62.3	19.1	6.0032	6.00338	6.003261	6.003261
3.5	−93.1	−31.4	2.3164	2.338	2.31676	2.316727
4.0	−211.6	−14.4	2.6989	2.695	2.7010	2.700719
5.0	132.1	−13.7	20.81	20.76	20.94	20.894501
6.0	52.4	−15.3	263.5	258.0	389.1	287.633460
7.0	34.0	−17.3	453.1	430.2	214.6	747.595333
8.0	25.9	−19.5	59.0	58.0	51.3	73.308294
9.0	21.4	−21.9	16.2	15.9	14.3	23.620704
10.0	18.5	−24.4	1.5	1.3	0.5	9.263055

As seen from the entries envisaged in Tables I and II, the convergence of the proposed method is quite rapid and the accuracy exceptionally good. Thus, for $N = 3$ the Padé approximants are practically as good as the exact solutions for s in the interval $-10 \leqslant s \leqslant 3$ and for $N \doteq 5$ this interval may be extended up to $s = 10$. For comparison, the radius of convergence of the Taylor expansion (22) and (23) is only 1.645. We have considered also other potential shapes finding convergence rate and accuracy very much the same as that exemplified above.

5. Conditions for the existence of a bound state

The number of bound states in a potential may be directly counted via numerical integration of the wave equation to find the corresponding eigenenergies. Regrettably, this procedure is rather laborious as usually a large number of integrations is being required. An alternative procedure [5] makes use of the properties of the scattering length and reduces to the evaluation of the poles in $a(s)$. To be more specific, the necessary and sufficient condition that a potential of a given strength s will support a bound state is

$$s \geqslant s_1$$

where s_1 is the nearest to zero pole in $a(s)$ (generally, $s \geqslant s_n$ is the condition for the existence of n levels). Thus, knowing s_1 one can answer immediately the question whether the potential supports a bound state, without the necessity to solve the associated and more difficult eigenvalue problem. We are now going to show that the Padé method just described provides an extremely economical way to determine s_1 with a high accuracy.

The poles of $a(s)$ in the Padé method are obtained as the zeros of $Q^{[N]}(s)$, where the latter quantity is given by the expressions (10) and (12) with $f_j \equiv a_j$. We denote the Padé approximations to s_1 by $s_1^{[N]}$, i. e.

$$Q^{[N]}(s_1^{[N]}) = 0.$$

The solution of the above equation for the first and second Padé approximant may be immediately obtained in an analytic form, viz.

$$s_1^{[1]} = \frac{a_1}{a_2} = \frac{\int_0^\infty V(r)rdr \int_0^\infty V(x)x^2dx}{2\int_0^\infty V(r)rdr \int_0^r V(x)x^2dx}, \tag{28}$$

$$s_1^{[2]} = -(\sqrt{y^2-4x} + y)/(2x), \tag{29}$$

where

$$x = (a_2a_4 - a_3^2)/(a_1a_3 - a_2^2), \quad y = (a_2a_3 - a_1a_4)/(a_1a_3 - a_2^2).$$

It can be easily shown that $s_1^{[1]} > s_1$, i. e. the $s_1^{[N]}$ tend to s_1 from above. Indeed, expanding $a(s)$ given by (3) and (5) in powers of s around $s = 0$, one finds

$$\frac{a_1}{a_2} = \frac{1}{1 - \sum_{n=1}^{\infty} \frac{1}{z_n}}, \tag{30}$$

where we have employed the following sum rule derived in [1]

$$\sum_{n=1}^{\infty} \frac{1}{s_n} = 1. \tag{31}$$

Separating out in the above equation the $1/s_1$ term, we can use Eq. (31) to calculate s_1 with the result

$$s_1 = \frac{1}{1 - \sum_{n=1}^{\infty} \frac{1}{s_{n+1}}}. \tag{32}$$

As shown in [1], $s_{n+1} > z_n$ and in view of (28) and (30) one obtains

$$s_1^{[1]} = \frac{1}{1 - \sum_{n=1}^{\infty} \frac{1}{z_n}} > \frac{1}{1 - \sum_{n=1}^{\infty} \frac{1}{s_{n+1}}} = s_1$$

which proves our assertion. Thus, strictly speaking, the inequality

$$s \gtrless s_1^{[N]}$$

has to be regarded as a sufficient but not necessary condition for the existence of a bound state. On the other hand, the $s_1^{[N]}$ rapidly converge to s_1 and the above restriction is inessential in practical applications.

To illustrate the rate of convergence of the Padé scheme we have displayed in Table III the values of $s_1^{[1]}$, $s_1^{[2]}$, and s_1 calculated for six different potentials. The shapes considered

TABLE III

The values of $s_1^{[1]}$, $s_1^{[2]}$, and s_1 for the following potential shapes: square well (SW), cut-off Coulomb (CC), exponential (EX), Hulthén (HU), Yukawa (YU), and Gaussian (GA)

	SW	CC	EX	HU	YU	GA
$s_1^{[1]}$	1.25	1.5	1.6	1.9068	2.0	1.4142
$s_1^{[2]}$	1.23372	1.4460	1.4468	1.6486	1.6843	1.3422
s_1	1.23370	1.4458	1.4458	1.6449	1.6799	1.3420

were: square well, cut-off Coulomb, exponential, Hulthén, Yukawa and Gaussian. As seen from the presented results, the values of $s_1^{[2]}$ are quite close to s_1. Since the first three digits or better have been always reproduced, $s_1^{[2]}$ should be sufficient for all practical purposes. It should be emphasized that this remarkable accuracy is being obtained merely by calculating the first four coefficients given by the integrals (25).

6. Summary and conclusions

We have developed a very effective and accurate approximation scheme for evaluating the scattering length and the effective range as functions of the potential strength. The method is based on the Padé approximation (8)–(12) and the appropriate Taylor expansion coefficients (22) and (23) are obtained from the recurrencies (25) and (26). The latter have been obtained by applying the variable phase method. Judging from the considered examples, it is quite sufficient to take $N = 3$ to obtain 0.1 % accuracy in the physically interesting region $-3.0 \leqslant s \leqslant 3.0$. The Padé method is very efficient for the task of calculating the scattering length as a function of s; it reduces to the evaluation of six integrals.

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