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Finite difference solution of the partial-wave Schrödinger equation

MS STERN^{†‡} and A E A WARBURTON[§]

[‡] Centre for Computer Studies, University of Hull, Hull, UK

[§] Department of Applied Mathematics, University of Hull, Hull, UK

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Abstract. A method is developed for the numerical determination of bound states and the eigenvalues of the Lippmann–Schwinger kernel for any local interaction. The eigenvalues of the scattering kernel are analytically continued from negative energies to positive energies by means of Padé approximants. The method is applied to calculations on low energy neutron–proton scattering.

1. Introduction

In recent years there has been a considerable interest in the calculation of three-body scattering amplitudes via the Faddeev equations. In order to perform such calculations one must be able to compute two-particle scattering amplitudes both on and off the energy shell (Faddeev 1961, Lovelace 1964, Bierter and Dietrich 1967a, 1967b).

By expressing the partial-wave Schrödinger equation in finite difference form we have developed a method of determining binding energies and the eigenvalues of the Lippmann–Schwinger kernel for any local potential. A knowledge of the eigenvalues of the scattering kernel is usually required when the two-body off-shell partial-wave T matrix is evaluated from an eigenfunction expansion (Weinberg 1963, Wright and Scadron 1964, Warburton and Stern 1969).

In a previous paper (Warburton and Stern 1969) we presented a method of computing the eigenvalues $\eta(k^2)$ of the Lippmann–Schwinger kernel for local interactions of the form

$$V(r) = \sum_{n=-1}^{\infty} v_n r^n \quad (v_{-1} \neq 0). \quad (1.1)$$

(k^2 is the energy in the centre of mass frame.) The $\eta(k^2)$ were represented by asymptotic expansions at high energies and these expansions were summed by the use of Padé approximants at low energies. The method could only find those eigenvalues which possessed the Coulomb high energy limit

$$\eta(k^2) \simeq \frac{1}{k}. \quad (1.2)$$

In the case of potentials of the form (1.1) which are either purely attractive or purely

[†]Now at Nuclear Studies Section, Computing Branch, Central Electricity Generating Board, 85 Park Street, London SE1

repulsive all the $\eta(k^2)$ have this high energy behaviour. However, when interactions of the form (1.1) contain both attractive and repulsive regions, only one set of their eigenvalues possesses the high energy limit (1.2).

The finite difference solution of the Schrödinger equation, which will be described in the following sections, does not restrict us to potentials of the form (1.1) and eigenvalues with the high energy behaviour (1.2). It should enable us to determine bound states and the $\eta(k^2)$ (irrespective of any particular high energy behaviour) of any analytic local interaction.

In § 2 the partial-wave Schrödinger equation is expressed in finite difference form. The resulting equations enable us to find only approximate values of binding energies because the boundary condition at infinity cannot be exactly applied. In § 3 the Schrödinger equation is transformed in such a way that it is possible to impose both of the boundary conditions exactly in the resulting finite difference solution, thereby enabling bound states to be determined more accurately than with the method of § 2. The method of § 3 also enables us to compute the $\eta(k^2)$ at negative energies. Numerical results are presented for various Yukawa and exponential potentials.

In § 4 the negative energy η (as determined by the method of § 3) are fitted by means of Padé approximants. These approximants are then used to analytically continue the eigenvalues to positive energies through the upper half k^2 plane.

In § 5 we apply the techniques developed in the previous two sections to calculations on low energy neutron-proton scattering in the triplet and singlet S states.

2. The finite difference solution

Binding energies and the $\eta(k^2)$ are determined from the partial-wave Schrödinger equation

$$\frac{d^2u}{dr^2} + \left(k^2 - \frac{l(l+1)}{r^2} - \frac{V(r)}{\eta(k^2)} \right) u = 0 \quad (2.1)$$

which is subject to the boundary conditions

$$u(r) \simeq r^{l+1} \quad \text{as } r \rightarrow 0$$

and (2.2)

$$u(r) \simeq \exp(ikr) \quad \text{as } r \rightarrow \infty$$

where we take $\text{Im } k \geq 0$, corresponding to the k^2 plane cut along the positive real axis.

By setting

$$r_n = nh \quad u_n = u(r_n) \quad \text{for } n = 0, 1, 2, 3, \dots \quad (2.3)$$

where h is small (note that $u_0 = 0$) we obtain

$$u'(r_n) \simeq \frac{u_{n+1/2} - u_{n-1/2}}{h} + O(h^2)$$

and (2.4)

$$u''(r_n) \simeq \frac{u_{n+1} - 2u_n + u_{n-1}}{h^2} + O(h^2)$$

Thus, by substituting (2.3) and (2.4) into equation (2.1) we find that the differential equation is reduced to an infinite system of homogeneous linear equations

$$-\frac{u_{n-1}}{h^2} + \left(\frac{V(r_n)}{\eta(k^2)} + \frac{2}{h^2} + \frac{l(l+1)}{r_n^2} \right) u_n - \frac{u_{n+1}}{h^2} = k^2 u_n \tag{2.5}$$

where $n = 1, 2, 3, \dots$. Obviously, it is a simple matter to impose the boundary condition at the origin since $u_0 = 0$, but, on the other hand, the second of the boundary conditions (2.2) can only be satisfied approximately when the system (2.5) is truncated at $n = M$ for M finite and sufficiently large. The assumption that the wavefunction vanishes at large r is a fairly good approximation at negative energies, that is, when k is restricted to the positive imaginary axis in the complex k plane.

For specified values of M and h we can employ the system of equations (2.5) to determine the energy eigenvalues k^2 of the potential $V(r)/\eta(k^2)$ by solving for the eigenvalues of the tridiagonal symmetric matrix formed by the coefficients of u_{n-1} , u_n , and u_{n+1} on the left hand side.

Now $\eta(k^2) = 1$ whenever an attractive potential $V(r)$ forms a physical bound state with energy $k^2 \leq 0$. Hence, any physical energy eigenvalues yielded by the system of equations (2.5) will be real and negative whilst all unphysical values will be real and positive definite (since a real symmetric matrix has only real eigenvalues). In tables 1 and 2 we present results for the S wave bound state values of k^2 obtained from equations (2.5), with various values of the step length h and order of matrix M , for a few attractive

Table 1. S wave bound state values of k^2 for the potential $V(r) = A \exp(-r)/r$, as determined from the finite difference solution (2.5) with $h = 0.1$. M gives the order of the matrix and N labels the bound states.

A	$M = 60$		$M = 100$		$M = 200$	
	$N = 1$	$N = 2$	$N = 1$	$N = 2$	$N = 1$	$N = 2$
-3.816632	-0.9740	---	-0.9741	---	-0.9741	---
-5.868286	-3.8391	---	-3.8391	---	-3.8391	---
-7.896615	-8.4679	-0.0459	-8.4679	-0.0800	-8.4679	-0.0827
-9.914714	-14.7040	-0.5231	-14.7040	-0.5253	-14.7040	-0.5253

Table 2. S wave bound state values of k^2 for the potential $V(r) = A \exp(-r)/r$, as determined from the finite difference solution (2.5) with $h = 0.05$. M gives the order of the matrix and N labels the bound states

A	$M = 60$		$M = 100$		$M = 200$	
	$N = 1$	$N = 2$	$N = 1$	$N = 2$	$N = 1$	$N = 2$
-3.816632	-0.9595	---	-0.9928	---	-0.9934	---
-5.868286	-3.9577	---	-3.9583	---	-3.9583	---
-7.896615	-8.8589	---	-8.8589	-0.0135	-8.8589	-0.0889
-9.914714	-15.6470	-0.3598	-15.6470	-0.5536	-15.6470	-0.5624

Yukawa potentials of the form $V(r) = A \exp(-r)/r$. These results can be compared with the exact binding energies, displayed in table 3, which were obtained by means of the Padé approximant method described in our previous paper (Warburton and Stern

1969). It is immediately obvious that the results obtained from the matrix eigenvalue method described above are only approximations to the exact bound states. The errors arise mainly from the fact that the boundary condition at infinity is not applied exactly when the system of linear equations (2.5) is truncated to finite order M .

Table 3. Exact S wave bound state values of k^2 for the potential $V(r) = A \exp(-r)/r$, N labels the bound states

N	A			
	—	—	—	—
1	-3.816632	-5.868286	-7.896615	-9.914714
2	-1.0000	-4.0000	-9.0000	-16.0000
2	—	—	-0.0943	-0.5754

In the next section equation (2.1) will be transformed in such a way that it will be possible to impose both of the boundary conditions (2.2) exactly in the resulting finite difference scheme, thereby enabling bound states to be determined more accurately than with the method developed in this section.

3. Transformation of the Schrödinger equation

The transformation

$$r = \frac{x}{1-x} \tag{3.1}$$

maps the interval $0 \leq r \leq \infty$ on to the interval $0 \leq x \leq 1$. The partial-wave Schrödinger equation (2.1) takes the form

$$(1-x)^4 \frac{d^2u}{dx^2} - 2(1-x)^3 \frac{du}{dx} + \left(k^2 - l(l+1) \frac{(1-x)^2}{x^2} - \frac{V(x)}{\eta(k^2)} \right) u = 0 \tag{3.2}$$

which satisfies the boundary conditions

$$u = 0 \text{ at } x = 0 \text{ and } x = 1. \tag{3.3}$$

We shall now establish a finite difference solution of this differential equation by setting

$$x_n = nh \quad u_n = u(x_n) \quad \text{for } n = 0, 1, 2, \dots, M+1$$

so that

$$h = \frac{1}{M+1} \quad u_0 = 0 = u_{M+1}. \tag{3.4}$$

We immediately see that both of the boundary conditions (3.3) have been applied exactly in contrast to the situation that arose in the previous section. The first and second derivatives of the wavefunction at the point x_n are given by

$$u'(x_n) \simeq \frac{u_{n+1/2} - u_{n-1/2}}{h} + O(h^2) \simeq \frac{u_{n+1} - u_{n-1}}{2h} + O(h^2)$$

and

$$u''(x_n) \simeq \frac{u_{n+1} - 2u_n + u_{n-1}}{h^2} + O(h^2). \tag{3.5}$$

By substituting (3.4) and (3.5) into equation (3.2) we obtain the finite system of homogeneous linear equations

$$\begin{aligned} &\frac{(1-x_n)^3(x_n-1-h)}{h^2}u_{n-1} + \left(\frac{V(x_n)}{\eta(k^2)} + \frac{2(1-x_n)^4}{h^2} + \frac{l(l+1)(1-x_n)^2}{x_n^2} \right) u_n \\ &+ \frac{(1-x_n)^3(x_n-1+h)}{h^2}u_{n+1} = k^2u_n \end{aligned} \tag{3.6}$$

where $n = 1, 2, 3, \dots, M$. Once again the energy eigenvalues k^2 of the interaction $V/\eta(k^2)$ are to be computed by solving the matrix eigenvalue problem but on this occasion the matrix of coefficients on the left hand side of (3.6) is nonsymmetric. It should be noted that the finite difference solution (3.6) is a more accurate representation of the Schrödinger equation than the solution (2.5) because no truncation of the system of linear equations has occurred in (3.6). From (3.4) it can be seen that the step length in (3.6) depends on the order of the matrix used to determine the energy eigenvalues whilst in (2.5) the step length is a free parameter.

In table 4 we present results for the S wave bound states of the Yukawa potentials considered in the previous three tables (setting η equal to unity). It can be seen that these results are much closer to the exact bound states than those obtained from equations (2.5).

Table 4. S wave bound state values of k^2 for the potential $V(r) = A \exp(-r)/r$, as determined from the finite difference solution (3.6). M gives the order of the matrix and N labels the bound states

A	$M = 60$		$M = 100$		$M = 200$	
	$N = 1$	$N = 2$	$N = 1$	$N = 2$	$N = 1$	$N = 2$
-3.816632	-1.0005	-	-1.0002	-	-1.0001	-
-5.868286	-3.9997	-	-3.9999	-	-4.0000	-
-7.896615	-8.9944	-0.0949	-8.9980	-0.0945	-8.9995	-0.0944
-9.914714	-15.9800	-0.5771	-15.9930	-0.5761	-15.9980	-0.5756

Of course, one should use the Padé approximant method developed in our previous paper (Warburton and Stern 1969) to locate bound states of Yukawa potentials and of other interactions of the form (1.1) (provided they possess attractive cores) because it is more accurate and very much faster than the finite difference method. The latter approach can be adopted when the former method cannot be applied. One such case is the exponential potential which is not of the form (1.1). In tables 5 and 6 we display S wave and P wave bound state values of k^2 for various exponential potentials of the form $V(r) = A \exp(-r)$. From these two tables and the previous one it can be seen that equations (3.6) yield results of at least three significant figure accuracy with matrices of order $M = 60$ to 100. Matrices of order 200 do, of course, lead to results of higher accuracy.

Table 5. S wave bound state values of k^2 for the potential $V(r) = A \exp(-r)$, as determined from the finite difference solution (3.6). M indicates the order of the matrix and N labels the bound states

A	$M = 60$		$M = 100$		$M = 200$	
	$N = 1$	$N = 2$	$N = 1$	$N = 2$	$N = 1$	$N = 2$
-2	-0.02005	—	-0.01998	—	-0.01995	—
-4	-0.31708	—	-0.31682	—	-0.31672	—
-6	-0.82358	—	-0.82315	—	-0.82297	—
-8	-1.4583	-0.00208	-1.4577	-0.00199	-1.4574	-0.00194
-9	-1.8112	-0.02481	-1.8105	-0.02448	-1.8102	-0.02434
-10	-2.1837	-0.07055	-2.1829	-0.06997	-2.1825	-0.06972

Table 6. P wave bound state values of k^2 for the potential $V(r) = A \exp(-r)$, as determined from the finite difference solution (3.6). M indicates the order of the matrix

A	$M = 60$	$M = 100$	$M = 200$
-8	-0.07607	-0.07584	-0.07574
-9	-0.19166	-0.19132	-0.19117
-10	-0.33475	-0.33431	-0.33412

In passing, we would like to point out that it has been shown (Massey and Mohr 1935, Stern 1969, pp 50–3) that the exact S wave bound states of the attractive exponential potential $V(r) = -A \exp(-\mu r)$, with $A > 0$, can be found from the roots of the equation

$$J_{-\nu} \left(\frac{2A^{1/2}}{\mu} \right) = 0 \quad (3.7)$$

where the left hand side is a Bessel function of order $-\nu = -2ik/\mu$.

The finite difference scheme (3.6) can also be employed to compute the eigenvalues $\eta(k^2)$ of a potential $V(r)$. The procedure is as follows. By substituting various real values of η into the system of equations we can determine whether there are any energy eigenvalues $k^2 (\leq 0)$ for the interaction $V(r)/\eta$. After a sufficient number of points have been found in the (η, k^2) plane, where k^2 is real and negative, the curve passing through these points can be fitted by means of Padé approximants, as described in the following section. These approximants can then be used to analytically continue the $\eta(k^2)$ of the potential under consideration from negative energies to positive energies through the upper half k^2 plane.

4. Curve fitting and analytic continuation by Padé approximants

It is supposed that a function $f(z)$, which is known to be finite at $z = 0$, has the asymptotic behaviour

$$f(z) \simeq z^{-t} \quad (t = 0, 1, 2, 3, \dots) \quad (4.1)$$

where $z = X + iY$. The function can then be represented by $[n + t, n]$ Padé approximants (Baker 1965)

$$f(z) \simeq \frac{P_n(z)}{Q_{n+t}(z)} = \frac{\sum_{m=0}^n p_m z^m}{\sum_{m=0}^{n+t} q_m z^m} \tag{4.2}$$

in which it is convenient to adopt the arbitrary normalization

$$q_0 = 1. \tag{4.3}$$

If the value of $f(z)$ is known at $(2n + t + 1)$ points on the real axis, we can set

$$f_j = f(X_j) \simeq \frac{\sum_{m=0}^n p_m X_j^m}{\sum_{m=0}^{n+t} q_m X_j^m} \tag{4.4}$$

where $j = 1, 2, 3, \dots, 2n + t + 1$. Thus, the coefficients p_m and q_m can be determined from the system of $(2n + t + 1)$ linear equations

$$\sum_{m=0}^n X_j^m p_m - f_j \sum_{m=1}^{n+t} X_j^m q_m = f_j. \tag{4.5}$$

After the polynomial coefficients have been found the function can be analytically continued from the real axis into the complex plane by means of the approximants (4.2) because the latter preserve analytic properties of functions such as poles, zeros, and cuts.

We shall employ the results of the previous section and those obtained so far in this section for the purpose of computing $\eta(k^2)$ at both positive and negative energies. The accuracy of the method can be tested on the attractive Yukawa potential $V(r) = -\exp(-r)/r$, for which results are already known (Warburton 1966, Warburton and Stern 1969, Stern 1969). The eigenvalues of this interaction do, of course, exhibit the high energy limit (1.2). Tables 7 and 8 display S wave and P wave values of k determined

Table 7. S wave values of k determined as a function of η from the finite difference solution (3.6) with a matrix of order 60 for the potential $V(r) = -\exp(-r)/r$. N labels the order of eigenvalue

η	$N = 1$	$N = 2$		$N = 3$	
	$-ik$	η	$-ik$	η	$-ik$
0.02	23.537	0.01	22.587	0.01	13.677
0.04	11.461	0.02	10.523	0.02	5.5511
0.06	7.3445	0.03	6.4258	0.03	2.8695
0.08	5.2789	0.04	4.3799	0.04	1.5621
0.10	4.0397	0.05	3.1598	0.05	0.80397
0.12	3.2149	0.06	2.3532	0.06	0.32040
0.14	2.6271	0.07	1.7828		
0.16	2.1874	0.08	1.3599		
0.18	1.8466	0.09	1.0352		
0.20	1.5748	0.10	0.77917		
0.22	1.3533	0.11	0.57290		
0.24	1.1694	0.12	0.40394		
0.26	1.0145	0.13	0.26363		
0.28	0.88224	0.14	0.14583		
0.30	0.76814				
0.32	0.66877				

Table 8. P wave values of k determined as a function of η from the finite difference solution (3.6) with a matrix of order 60 for the potential $V(r) = -\exp(-r)/r$. N labels the order of eigenvalue

$N = 1$		$N = 2$	
η	$-ik$	η	$-ik$
0.005	49.973	0.005	31.878
0.010	23.241	0.010	13.935
0.015	14.760	0.015	8.2963
0.020	10.562	0.020	5.5200
0.025	8.0535	0.025	3.8692
0.030	6.3851	0.030	2.7756
0.035	5.1950	0.035	1.9971
0.040	4.3030	0.040	1.4123
0.045	3.6092	0.045	0.95165
0.050	3.0537	0.050	0.56785
0.055	2.5984		
0.060	2.2178		
0.065	1.8943		
0.070	1.6152		
0.075	1.3710		
0.080	1.1543		
0.085	0.95938		
0.090	0.78112		

as a function of η from the finite difference solution (3.6) with a matrix of order 60. These results can be fitted by $[n, n - 1]$ Padé approximants in the variable $K = ik$ in order to analytically continue the various $\eta(k^2)$ from negative energies to positive energies. In tables 9 and 10 we present results for the eigenvalues computed at both positive and negative energies; in the S wave case [8, 7] approximants were used for the first eigenvalue, [7, 6] for the second, and [3, 2] for the third whilst in the P wave case [9, 8] approximants were employed for the first eigenvalue and [5, 4] for the second. In each case we observe that there is good agreement with previously obtained results, and therefore we feel confident that the method is reliable for finding eigenvalues which do not possess the Coulomb high energy limit (1.2).

Table 9. The first three S wave eigenvalues computed by fitting $[n, n - 1]$ Padé approximants in the variable $K = ik$ to the results of table 7 for the potential $V(r) = -\exp(-r)/r$

k	$N = 1$			$N = 2$			$N = 3$		
	Re $\eta(k^2)$	Im $\eta(k^2)$	$\eta(-k^2)$	Re $\eta(k^2)$	Im $\eta(k^2)$	$\eta(-k^2)$	Re $\eta(k^2)$	Im $\eta(k^2)$	$\eta(-k^2)$
0.0	0.5949	0	0.5949	0.1552	0	0.1552	0.0697	0	0.0697
0.1	0.5837	0.0780	0.5252	0.1541	0.0117	0.1444	0.0695	0.0036	0.0663
0.2	0.5529	0.1468	0.4709	0.1511	0.0227	0.1352	0.0688	0.0071	0.0633
0.5	0.4108	0.2630	0.3612	0.1344	0.0484	0.1141	0.0647	0.0164	0.0558
1.0	0.2299	0.2732	0.2620	0.1013	0.0678	0.0912	0.0545	0.0260	0.0469
2.0	0.0918	0.2002	0.1704	0.0569	0.0684	0.0658	0.0369	0.0315	0.0359
5.0	0.0184	0.0958	0.0838	0.0158	0.0428	0.0363	0.0132	0.0250	0.0215

Table 10. The first two P wave eigenvalues computed by fitting $[n, n-1]$ Padé approximants in the variable $K = ik$ to the results of table 8 for the potential $V(r) = -\exp(-r)/r$

k	$N = 1$			$N = 2$		
	$\text{Re } \eta(k^2)$	$\text{Im } \eta(k^2)$	$\eta(-k^2)$	$\text{Re } \eta(k^2)$	$\text{Im } \eta(k^2)$	$\eta(-k^2)$
0.0	0.1107	0	0.1107	0.0566	0	0.0566
0.1	0.1116	0.0005	0.1096	0.0571	0.0002	0.0561
0.2	0.1140	0.0019	0.1074	0.0583	0.0012	0.0550
0.5	0.1229	0.0169	0.0986	0.0607	0.0084	0.0509
1.0	0.1093	0.0524	0.0839	0.0554	0.0209	0.0444
2.0	0.0621	0.0665	0.0633	0.0384	0.0301	0.0350
5.0	0.0165	0.0432	0.0360	0.0137	0.0248	0.0213

We shall now turn our attention to the S wave eigenvalues of the exponential potential $V(r) = -\exp(-r)$. It has been shown (Stern 1969) that these eigenvalues have the high energy behaviour

$$\eta(k^2) \simeq \frac{1}{k^2}. \tag{4.6}$$

Table 11 contains values of k determined as a function of η from the finite difference solution (3.6) with a matrix of order 100. These results have been fitted by $[n, n-2]$

Table 11. S wave values of k determined as a function of η from the finite difference solution (3.6) with a matrix of order 100 for the potential $V(r) = -\exp(-r)$. N labels the order of eigenvalue

η	$N = 1$		$N = 2$	
	$-ik$	η	$-ik$	η
0.01	7.5030	0.01	5.6647	
0.02	4.8513	0.02	3.2246	
0.03	3.7019	0.03	2.1890	
0.04	3.0278	0.04	1.5915	
0.05	2.5739	0.05	1.1948	
0.06	2.2427	0.06	0.90895	
0.07	1.9880	0.07	0.69163	
0.08	1.7846	0.08	0.51997	
0.09	1.6176	0.09	0.38045	
0.10	1.4775	0.10	0.26451	
0.11	1.3578	0.11	0.16644	
0.12	1.2542	0.12	0.082292	
0.13	1.1634	0.13	0.0098471	
0.14	1.0830			
0.15	1.0113			
0.16	0.94682			
0.17	0.88844			
0.18	0.83529			
0.19	0.78666			

approximants (in the variable $K = ik$) which have yielded the positive and negative energy values of $\eta(k^2)$ displayed in table 12; [10, 8] approximants were used for the first eigenvalue and [7, 5] for the second.

Table 12. The first two S wave eigenvalues computed by fitting $[n, n-2]$ Padé approximants in the variable $K = ik$ to the results of table 11 for the potential $V(r) = -\exp(-r)$

k	$N = 1$			$N = 2$		
	Re $\eta(k^2)$	Im $\eta(k^2)$	$\eta(-k^2)$	Re $\eta(k^2)$	Im $\eta(k^2)$	$\eta(-k^2)$
0.0	0.6900	0	0.6900	0.1311	0	0.1311
0.1	0.6537	0.1689	0.5450	0.1299	0.0148	0.1178
0.2	0.5603	0.2993	0.4444	0.1258	0.0288	0.1064
0.5	0.2315	0.4033	0.2724	0.1019	0.0608	0.0813
1.0	-0.0035	0.2630	0.1517	0.0543	0.0770	0.0565
2.0	-0.0512	0.0955	0.0695	0.0054	0.0564	0.0327
5.0	-0.0203	0.0154	0.0191	-0.0093	0.0158	0.0118

At $k = i\mu/4$ the S wave eigenvalues of the interaction $V(r) = -A \exp(-\mu r)$ have the exact values (Stern 1969, pp 50-3)

$$\eta\left(-\frac{\mu^2}{16}\right) = \frac{4A}{N^2 \pi^2 \mu^2} \quad (N = 1, 2, 3, \dots) \quad (4.7)$$

where N is the order of eigenvalue. This formula yields 0.4053 and 0.1013 for the first and second eigenvalues respectively when $A = \mu = 1$. The Padé approximants that were employed to compute the results in table 12 gave corresponding values of 0.4050 and 0.1014 at the same energy. We are therefore confident that the values of $\eta(k^2)$ presented in this table are accurate to at least three significant figures.

In the following section the methods developed in this section and the previous one will be employed to calculate the eigenvalues of interactions which change sign.

5. Neutron-proton scattering

A process that has attracted considerable interest, both theoretical and experimental, is low energy neutron-proton scattering. As the masses of the particles are large when compared with the energies and momentum transfers involved in the scattering experiments, one tries to represent the interaction between the nucleons by means of a non-relativistic central potential. We assume that the tensor force and spin-orbit interaction can be safely ignored at energies below 310 MeV, the pion production threshold.

For the triplet S state, Coester and Yen (1963) have proposed the double Yukawa potential

$$V(r) = \frac{4A \exp(-2\mu r)}{r} - \frac{A \exp(-\mu r)}{r} \quad (5.1)$$

($A > 0$) which has a repulsive core and an attractive outer region. The parameters A

and μ are determined from the experimentally measured scattering length a and effective range r_0 . When r is measured in fermi, $k^2 = 1$ corresponds to an energy of 41.5 MeV in the centre of mass frame (or 83 MeV in the laboratory frame). This interaction has an infinite number of repulsive eigenvalues with the high energy limit $\eta \simeq 1/k$ and an infinite number of attractive eigenvalues with the high energy behaviour $\eta \simeq 1/k^2$. We have determined the first eight repulsive eigenvalues (Warburton 1966, Stern 1969) by using the method developed in our previous paper (Warburton and Stern 1969) when $A = 42.48$ and $\mu = 2.307$. However, as mentioned earlier in this paper, that method cannot be employed to find the attractive eigenvalues which, therefore, will be computed with the aid of the equations derived in §§ 3 and 4.

It is well known that the deuteron has a binding energy of about 2.22 MeV ($k^2 = -0.05350$). By substituting the potential (5.1), with the values of A and μ specified in the previous paragraph, into the finite difference scheme (3.6) we find that matrices of order 60, 100, and 200 yield binding energies of $k^2 = -0.05397$, -0.05366 , and -0.05352 respectively for the deuteron. (The deuteron bound state is located by setting the first attractive $\eta(k^2)$ to unity in (3.6).)

We have employed the method developed in the previous two sections to calculate the first two repulsive and the first two attractive eigenvalues of the triplet S state interaction at both positive and negative energies. We find that the results, which are presented in tables 13 and 14, are in good agreement with those determined by other methods (Warburton 1966, Stern 1969).

Table 13. The first two repulsive eigenvalues of the triplet S state potential (5.1)

k	$N = 1$			$N = 2$		
	Re $\eta(k^2)$	Im $\eta(k^2)$	$\eta(-k^2)$	Re $\eta(k^2)$	Im $\eta(k^2)$	$\eta(-k^2)$
0.0	-12.33	0	-12.33	-3.01	0	-3.01
0.1	-12.33	-0.18	-12.15	-3.01	-0.01	-3.00
0.2	-12.34	-0.36	-11.97	-3.02	-0.02	-2.99
0.5	-12.38	-0.95	-11.41	-3.04	-0.06	-2.94
1.0	-12.35	-2.12	-10.53	-3.10	-0.15	-2.85
2.0	-11.26	-4.52	-9.06	-3.18	-0.52	-2.64
5.0	-6.12	-6.45	-6.31	-2.57	-1.39	-2.11

Table 14. The first two attractive eigenvalues of the triplet S state potential (5.1)

k	$N = 1$			$N = 2$		
	Re $\eta(k^2)$	Im $\eta(k^2)$	$\eta(-k^2)$	Re $\eta(k^2)$	Im $\eta(k^2)$	$\eta(-k^2)$
0.0	1.331	0	1.331	0.160	0	0.160
0.1	1.314	0.175	1.171	0.160	0.008	0.152
0.2	1.262	0.341	1.038	0.159	0.016	0.145
0.5	0.961	0.713	0.752	0.152	0.038	0.127
1.0	0.365	0.846	0.483	0.133	0.068	0.104
2.0	-0.126	0.468	0.248	0.082	0.098	0.074
5.0	-0.094	0.064	0.073	-0.007	0.066	0.034

We shall now turn our attention to the singlet S state potential (Mongan 1969)

$$V(r) = \frac{6484.2 \exp(-7\beta r) - 1650.6 \exp(-4\beta r) - 10.463 \exp(-\beta r)}{41.5\beta r} \quad (5.2)$$

where $\beta = 0.7$. This also has a repulsive core and an attractive outer region. ($k^2 = 1$ again corresponds to an energy of 41.5 MeV in the centre of mass frame.) The attractive and repulsive $\eta(k^2)$ of this interaction have the same high energy limits as the corresponding eigenvalues of the potential (5.1). The leading eigenvalues, computed at both positive and negative energies, are displayed in table 15. The results obtained for the first repulsive $\eta(k^2)$ are in close agreement with those found by using our earlier asymptotic expansion and Padé approximant method (Warburton and Stern 1969).

Table 15. The leading repulsive and attractive eigenvalues of the singlet S state potential (5.2)

k	Repulsive			Attractive		
	Re $\eta(k^2)$	Im $\eta(k^2)$	$\eta(-k^2)$	Re $\eta(k^2)$	Im $\eta(k^2)$	$\eta(-k^2)$
0.0	-15.86	0	-15.86	0.924	0	0.924
0.1	-15.86	-0.26	-15.60	0.908	0.127	0.809
0.2	-15.87	-0.52	-15.35	0.865	0.243	0.716
0.5	-15.86	-1.34	-14.59	0.650	0.476	0.520
1.0	-15.66	-2.86	-13.44	0.275	0.563	0.338
2.0	-14.16	-5.67	-11.54	-0.068	0.339	0.177
5.0	-7.91	-8.13	-8.07	-0.068	0.050	0.053

In future work we hope to combine the methods developed in this paper and in our previous one (Warburton and Stern 1969) in order to compute the off-shell scattering amplitudes of the nucleon-nucleon interactions (5.1) and (5.2) (and also possibly of other local potentials which change sign).

6. Conclusions

The numerical methods described in this paper are suitable for calculating all the eigenvalues of the Lippmann-Schwinger kernel (at both positive and negative energies) and binding energies for any analytic local potential and orbital angular momentum l . However, when dealing with interactions of the form (1.1) which are either purely attractive or purely repulsive, one should use our asymptotic expansion and Padé approximant approach (Warburton and Stern 1969) since it is more accurate and very much faster than the finite difference solution. Our previous results should also be employed to determine the set of $\eta(k^2)$ possessing the Coulomb high energy limit (1.2) when studying potentials of the form (1.1) which contain both attractive and repulsive regions. The finite difference method (combined with curve fitting and analytic continuation by Padé approximants) may then be used to find the eigenvalues which exhibit other high energy limits. It is hoped that we shall be able to combine the methods developed in this paper and our previous one (Warburton and Stern 1969) in order to evaluate the off-shell partial-wave T matrix for physically 'realistic' interactions such as (5.1) and (5.2).

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