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Extrapolation technique for solution of scattering integral equations

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Abstract. The Romberg extrapolation technique, widely used for the evaluation of integrals, is generalised and applied to solving integral equations in scattering theory. The proposed approach makes it possible to obtain accurate results with a very small number of mesh points and to control the error of the approximation. Typical examples of the calculation of phase shifts and singularities of the T matrix (i.e. of the energies of bound, virtual and resonance states) are presented.

1. Introduction

Since the advent of the Faddeev equations in the early 1960s (Faddeev 1960) the integral equation description of scattering processes has become increasingly popular. The integral equation approach has several advantages over the traditional description by differential equations. Among others, the following two are of great importance: first, the boundary conditions are already incorporated in the integral equation and need not be added separately as in the case of differential equations (this is very important for problems where three or more particles interact) and, second, there exist well developed very efficient methods for solving integral equations which are usually much more stable than their differential equation counterparts.

In this paper we restrict ourselves to one-channel problems. A typical example is the static exchange approximation of electron–hydrogen scattering (Mott and Massey 1965). The integral equation describing this process is

$$\begin{aligned} \psi_l(k, r) = & u_l(kr) + \int_0^\infty G_l(k, r, r') V_l(r') \psi_l(k, r') \, dr' \\ & + \int_0^\infty \int_0^\infty G_l(k, r, r') U_l(r', r'') \psi_l(k, r'') \, dr' \, dr'' \end{aligned} \quad (1)$$

where $u_l(kr)$ is the free-particle wavefunction regular at the origin, G_l is the free-particle Green function, V_l is the static (i.e. local) part of the interaction and U_l is the non-local part of the electron–hydrogen interaction caused by exchange of the electrons. The Green function G_l is a smooth function of r and r' but has a cusp at $r = r'$, where its first derivative is discontinuous. The explicit form of G_l is

$$G_l(k, r, r') = \begin{cases} u_l(kr)v_l(kr') & r' > r \\ u_l(kr')v_l(kr) & r > r' \end{cases} \quad (2)$$

where v_l is the free-particle wavefunction irregular at the origin and both functions u_l and v_l are assumed to be normalised so that their Wronskian is equal to unity.

To solve equation (1) a discretisation of the variables r and r' must be introduced. Let us denote for simplicity the integral kernel $G_l(V_l + U_l)$ of (1) as K_l and introduce a quadrature rule with mesh points $\{r_i\}_1^N$ and weights $\{W_i\}_1^N$. Equation (1) then reduces to an algebraic equation:

$$\psi_l^{(N)}(k, r_i) = u_l(kr_i) + \sum_{j=1}^N K_l(r_i, r_j) W_j \psi_l^{(N)}(k, r_j) \quad (3)$$

where we have added the superscript N to ψ_l to explicitly indicate its dependence on the total number of mesh points N .

The quantity of principal interest in the scattering theory is not the wavefunction ψ_l itself but the T matrix, which is defined as

$$T_l = \int_0^\infty \int_0^\infty u_l(kr) K_l(r, r') \psi_l(k, r') dr dr'. \quad (4)$$

As before we denote by $T_l^{(N)}$ the T -matrix value obtained by means of a quadrature using N mesh points.

It had been recognised a long time ago (Fraser 1961, Stern 1977) that the application of a numerical quadrature over the full integration range would give rise to an undefined error because of the discontinuous first derivative of the Green function at $r = r'$. Recently Oza and Callaway (1987) implemented successfully the Newton-Cotes quadrature formulae of high order with proper allowance for the discontinuity. Here we shall propose another way of avoiding the discontinuity problem, namely to use the trapezoidal rule (here all mesh points are the endpoints of the quadrature, and therefore the error is strictly under control) together with an extrapolation technique.

2. Extrapolation technique

The Romberg extrapolation technique is based on the expansion (Stroud 1974)

$$\int_a^b f(x) dx = \sum_{i=0}^N W_i f(a + ih) + \alpha_2 h^2 + \alpha_4 h^4 + \dots \\ = T(h) + R(h). \quad (5)$$

Here $T(h)$ is an approximation of the integral obtained by the trapezoidal rule with the constant grid size h ,

$$W_i = \begin{cases} h/2 & i = 1, N \\ h & i = 2, 3, \dots, N-1 \end{cases} \quad N = (b-a)/h$$

are the weights and $R(h)$ is the remainder, which for small h behaves as h^2 . The essence of the Romberg extrapolation technique is to calculate two approximations to the integral, $T(h)$ and $T(h/2)$, and to construct from them a new approximation

$$\int_a^b f(x) dx = \frac{4T(h/2) - T(h)}{3} + R_1(h) \quad (6)$$

where the remainder $R_1(h)$ behaves as h^4 for small h . The calculation is then repeated with grid sizes $h/4$, $h/8$, $h/16$, etc, with the error of approximation decreasing as h^6 , h^8 , etc, until convergence is eventually reached.

It is not clear *a priori* whether this approach can be applied to the calculation of the T -matrix elements in the form (4). The calculation of the T -matrix elements differs from the calculation of an integral in two respects. The first problem is that the integrand itself depends on the number of mesh points N :

$$T_i^{(N)} = \sum_{i=0}^N \sum_{j=0}^N u_i(kr_i) K_i(r_i, r_j) \psi_i^{(N)}(k, r_j) W_i W_j. \tag{7}$$

This means that, by changing the number of mesh points N in (3), we generally obtain different values of the solution (i.e. of the function to be integrated) at any point common to both sets of mesh points, i.e.

$$\psi_i^{(N)}(k, r_i) \neq \psi_i^{(2N)}(k, r_i).$$

The second problem is related to the spacing of the mesh points. The integration points are assumed to be spaced equidistantly in the Romberg approach, whereas in many physical situations the meshes must be chosen to be finer at smaller radial distances, where the interactions are usually stronger. What grid size h should be used in (5) in such a case?

It is the purpose of this paper to demonstrate that the Romberg extrapolation technique, combined with variable grid sizes, constitutes a simple and very efficient means of calculation of T -matrix elements with high accuracy and controlled error.

3. Results

First we shall treat the case of local forces, i.e. $U_l = 0$ in (1). For simplicity we restrict ourselves to the case $l = 0$ and omit all unnecessary subscripts. The Green function now takes the explicit form

$$G_0(k; r, r') = \begin{cases} -\frac{1}{k} \sin kr \cos kr' & r' > r \\ -\frac{1}{k} \cos kr \sin kr' & r > r'. \end{cases} \tag{8}$$

Equation (1), which is of Fredholm type, can easily be transformed to a Volterra-type equation:

$$\varphi(k, r) = \frac{\sin kr}{k} - \frac{1}{k} \int_0^r (\cos kr \sin kr' - \sin kr \cos kr') V(r') \varphi(k, r') dr' \tag{9}$$

i.e.

$$\varphi(k, r) = \frac{\sin kr}{k} + \int_0^r g(k; r, r') V(r') \varphi(k, r') dr'$$

where

$$g(k; r, r') = G_0(k; r, r') + (1/k) \sin kr \cos kr'. \tag{10}$$

The solution $\psi(k, r)$ of (1) is expressed in terms of $\varphi(k, r)$ as

$$\psi(k, r) = \frac{\varphi(k, r)}{1 + \int_0^\infty \cos kr V(r) \varphi(k, r) dr} \tag{11}$$

and the T -matrix element (more precisely, the K -matrix element in this case) as

$$T(k) = \frac{\int_0^\infty \sin kr V(r) \varphi(k, r) dr}{1 + \int_0^\infty \cos kr V(r) \varphi(k, r) dr}. \quad (12)$$

This quantity relates to the phase shift as

$$T(k) = -\tan \delta(k). \quad (13)$$

The real principal-value Green function in (8) can be used only for real energies. For complex energies (i.e. for the calculation of resonances) this function must be replaced by

$$G_0(k, r, r') = \begin{cases} -\frac{1}{k} \sin kr \exp(ikr') & r' > r \\ -\frac{1}{k} \sin kr' \exp(ikr) & r > r'. \end{cases} \quad (14)$$

Then (12) defines the T matrix. Equation (9) is of the Volterra type. After discretising the variables we obtain an algebraic equation which is very easy to solve because the resulting matrix is triangular. To test this approach we have calculated the s -wave phase shifts for various potentials with increasing degree of complexity.

3.1. Exponential potential

The potential

$$V(r) = -2 \exp(-r) \quad (15)$$

had been previously investigated by many authors and the result of a variational calculation for $k = 0.35$ is (Lucchese *et al* 1983)

$$\tan \delta = 9.091\ 8095.$$

The results are summarised in table 1. The entries in the column headed '1.0' were obtained by resorting to the equidistant partition of the interval (0, 24) and N is the number of mesh points used for the extrapolation. This means that, for example, the value in the third row of this column has been obtained using 20, 39 and 77 mesh points (i.e. grid sizes $h = \frac{24}{19}$, $\frac{24}{39}$ and $\frac{24}{76}$, respectively). The results demonstrate very fast convergence to the exact value.

Table 1. Extrapolated value of $\tan \delta(k)$ at $k = 0.35$ for the exponential potential (15). N denotes the number of mesh points and Q is the parameter in (16) which determines the distribution of the mesh points. For $Q > 1$ the grid spacings are finer near the origin.

N	Q				
	1.0	1.5	2.0	3.0	4.5
20	11.195 327 0	10.761 037 3	11.008 306 3	11.905 779 3	14.403 323 0
39	11.659 513 4	9.092 824 23	9.083 362 61	9.083 623 79	9.079 796 06
77	9.047 731 61	9.092 857 11	9.091 816 98	9.091 820 73	9.091 824 92
153	9.091 207 99	9.091 825 24	9.091 809 47	9.091 809 47	9.091 809 46
305	9.091 812 36	9.091 810 04	9.091 809 48	9.091 809 48	9.091 809 48
609	9.091 809 48	9.091 809 50	9.091 809 48	9.091 809 48	9.091 809 48

The other columns of this table are designed to test the applicability of the extrapolation technique in the case of non-equidistant mesh points. The parameter Q determines the distribution of the mesh points as follows:

$$r_i = R_{\max} \left(\frac{i-1}{N-1} \right)^Q \quad i = 1, 2, \dots, N. \quad (16)$$

For $Q = 1$ the grid size is constant, whereas for $Q > 1$ the grid becomes finer near the origin. For example, for $Q = 2$ one-half of the meshes fall on the interval $(0, 0.25R_{\max})$. All these calculations confirm the hypothesis that the extrapolation technique also converges in the case of non-equidistant mesh points. This makes it possible to get very precise results using a very small number of mesh points. For example, the value of the phase shift obtained with $N = 20, 39$ and 77 mesh points and $Q = 2$ is correct to six significant figures, and that obtained with $N = 20, 39, 77$ and 153 points is correct to almost nine figures. Moreover, this convergence rate remains unchanged over a broad range of Q .

3.2. Yukawa potential

The Yukawa potential

$$V(r) = -2 \exp(-r)/r$$

has also been treated recently by Oza and Callaway (1987). The results of a phase-shift calculation for various energies and $Q = 2$ are summarised in table 2. Again we find very fast convergence in a very broad energy range.

Table 2. Extrapolated values of the s -wave phase shift δ for the Yukawa potential (18). N denotes the number of mesh points and E is the energy.

N	E					
	0.01	0.1	1.0	2.0	5.0	10.0
8	2.693 706 20	2.022 945 88	1.283 464 44	1.110 923 23	0.822 530 951	0.952 164 058
15	2.440 036 64	1.701 878 65	1.073 940 97	0.913 020 334	0.750 080 863	0.540 020 249
29	2.439 847 95	1.722 695 45	1.092 957 73	0.934 106 330	0.743 164 335	0.620 025 113
57	2.439 654 18	1.722 225 50	1.092 441 45	0.933 424 531	0.744 235 37	0.617 367 418
113	2.439 656 17	1.722 209 50	1.092 445 56	0.933 431 301	0.744 217 11	0.617 299 494
255	2.439 656 17	1.722 209 49	1.092 445 55	0.933 431 282	0.744 217 14	0.617 301 385

3.3. Reid soft-core singlet potential

This potential (Reid 1968), which describes the nucleon-nucleon interaction, consists of three Yukawa-type terms and is very difficult to handle because its repulsive part is very strong. In order to also test other distributions of mesh points we used in this case a grid with exponentially increasing points

$$r_i = R_{\max} \left[\exp \left(Q \frac{i-1}{N-1} \right) - 1 \right] (\exp Q - 1)^{-1} \quad i = 1, 2, \dots, N. \quad (17)$$

The results for $E_{\text{lab}} = 24$ MeV are shown in table 3.

Table 3. Extrapolated values of the s -wave phase shift δ for the Reid soft-core singlet potential at $E_{\text{lab}} = 24$ MeV. N denotes the number of mesh points and Q is the parameter in (17) determining the distribution of the mesh points. For $Q = 1$ the mesh points are equidistant, and for $Q > 1$ the grid spacings are finer near the origin.

N	Q				
	1	2	4	6	9
20	1.078 164 444	0.771 374 708	0.736 141 893	0.744 214 275	0.775 019 594
39	0.647 869 531	0.717 767 183	0.717 884 289	0.717 759 870	0.717 115 867
77	0.722 291 586	0.717 905 330	0.718 013 761	0.718 016 109	0.718 011 013
153	0.717 892 620	0.718 012 928	0.718 013 342	0.718 013 311	0.718 013 505
305	0.718 012 902	0.718 013 305	0.718 013 344	0.718 013 344	0.718 013 343
609	0.718 013 320	0.718 013 344	0.718 013 344	0.718 013 344	0.718 013 344

3.4. Positron-hydrogen scattering in the static approximation

This problem is difficult because the incident positron polarises the atom and the resulting interaction is long ranged (Sarkar *et al* 1979):

$$V(r) = 2 \exp(-r)(1 + 1/r) - \alpha(r)/r^4 \quad (18)$$

where

$$\alpha(r) = 4.5 - \exp(-2r)(3/2r^5 + 3r^4 + 6r^3 + 9r^2 + 9r + 4.5).$$

The results for $k = 0.5$ and $R_{\text{max}} = 200$ are shown in table 4. The first column contains the non-extrapolated results obtained by equidistant partition of the integration range $(0, 200)$, and the results in the second column were again obtained without extrapolation but with a grid size which increased with the distance from the origin as r^4 . The extrapolated results are given in the last column of this table and are probably correct to all the significant figures shown. To achieve the same accuracy without extrapolation and with $h = \text{constant}$ one would have to use at least 100 000 mesh points.

Table 4. Extrapolated values of the s -wave phase shift for the potential (18) modelling positron-hydrogen elastic scattering. N is the number of mesh points.

N	$Q = 1$	$Q = 4$	$Q = 4$
	Non-extrapolated	Non-extrapolated	Extrapolated
20	0.006 0054	-0.045 7567	-0.045 7567
39	0.017 4396	-0.047 3526	-0.047 8846
77	0.179 241	-0.047 5183	-0.047 5528
153	0.013 9302	-0.047 5595	-0.047 5735
305	-0.035 1142	-0.047 5699	-0.047 5734
609	-0.044 5609	-0.047 5725	—
1217	-0.046 8254	-0.047 5732	—
2433	-0.047 3862	-0.047 5733	—
4865	-0.047 5261	-0.047 5734	—

3.5. Calculation of the *T*-matrix poles

The extrapolation technique described above can also be used for calculation of the *T*-matrix poles which, depending on their position in the complex *k* plane, correspond to bound, virtual or resonance states. The *T* matrix given by (12) has a pole if

$$1 + \int_0^\infty \cos krV(r)\varphi(k, r) dr = 0 \tag{19}$$

(here, for the calculation of φ we must use the complex Green function (14)). To find such a pole we must solve (9) for several energies in the vicinity of the pole and then vary *k* until (19) is satisfied. The results of the calculation of the energy E_v of a virtual state (singlet deuteron) for the Reid soft-core potential (Reid 1968) are given in table 5. The pattern of convergence for the triplet case, where a bound state (the deuteron) exists, is similar. Table 6 shows the results of calculation of a (complex) resonance energy in the $n+\alpha$ scattering problem, modelled by the Woods-Saxon potential (Kukulin *et al* 1983), in which two resonances (one narrow and one broad) have been computed.

3.6. Electron-hydrogen elastic scattering

As a final example of the extrapolation approach we take the much more fundamental problem of elastic scattering of electrons by hydrogen atoms in the static exchange approximation (Mott and Massey 1965). Here the non-local exchange interaction *U* is of fundamental importance and its presence makes this problem difficult to solve. Now, no transformation of the type (10) makes the kernel *K* triangular and other methods for solving (1) must be used. For this purpose we used the method of continued

Table 5. Extrapolated values of the energy of the virtual state (singlet deuteron) for the Reid soft-core potential. *N* is the number of mesh points.

<i>N</i>	E_v (MeV)
21	-0.024 3776
41	-0.100 1009
81	-0.119 5639
161	-0.121 6988
321	-0.121 7624
641	-0.121 7624

Table 6. Extrapolated energies *E* and widths Γ (in MeV) in $n+\alpha$ scattering. *N* is the number of mesh points.

<i>N</i>	E_r	Γ	E_r	Γ
21	0.912 2943	0.911 5573	1.679 1608	5.485 4995
41	0.832 6353	0.772 4977	1.662 7154	5.589 2748
81	0.836 9117	0.779 5086	1.663 8234	5.582 3361
161	0.836 8575	0.779 4177	1.663 8095	5.582 4229
321	0.836 8576	0.779 4178	1.663 8095	5.582 4229
641	0.836 8576	0.779 4178	1.663 8095	5.582 4229

Table 7. Extrapolated values of s -wave phase shifts for elastic scattering of electrons by hydrogen atoms in the static exchange approximation. N is the number of mesh points used at each extrapolation step. $R_{\max} = 12$.

N	E							
	0.01	0.09	0.25	0.49	0.76	1.0	2.0	5.0
8	2.3888	1.5036	1.0303	0.749 94	0.614 83	0.560 36	0.553 11	0.818 73
15	2.3964	1.5084	1.0307	0.743 41	0.600 91	0.541 98	0.505 79	0.470 40
29	2.3964	1.5086	1.0311	0.744 27	0.601 86	0.542 74	0.509 44	0.549 81
57	2.3964	1.5086	1.0311	0.744 27	0.601 86	0.542 77	0.509 35	0.544 86

Table 8. Extrapolated values of s -wave phase shifts for elastic scattering of electrons by hydrogen atoms in the static exchange approximation and $R_{\max} = 30$.

E	δ_0^+	δ_0^-
0.01	2.395 803 43	2.907 599 82
0.09	1.508 099 37	2.461 128 28
0.25	1.031 498 28	2.070 066 64
0.49	0.744 148 07	1.748 819 59
0.76	0.601 717 36	1.527 218 41
1.0	0.542 894 64	1.390 519 78
2.0	0.509 320 20	1.075 615 42
5.0	0.544 930 79	0.763 915 79

fractions which we proposed some time ago (Horáček and Sasakawa 1983, 1984, 1985). This method is iterative, but its convergence is guaranteed and usually a very small number of iterations (three or four) gives quite accurate results. The results are summarised in table 7. The phase shifts have been calculated with $R_{\max} = 12$. This value is sufficiently large for four-figure accuracy. In order to obtain a higher accuracy a larger value of R_{\max} must be used. The phase shifts in table 8 have been obtained with $R_{\max} = 30$ and are probably correct to all figures.

4. Conclusion

In conclusion we can state that the application of the Romberg extrapolation technique with variable grids to the solution of integral equations represents a very powerful tool for calculation of not only phase shifts but also of bound, virtual and resonance states. The generalisation to off-shell scattering is straightforward, and very accurate values of the off-shell T -matrix elements can be obtained with a very small number of mesh points.

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