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Simple numerical solution of the partial-wave Lippmann–Schwinger equation

M S STERN†

Centre for Computer Studies, University of Hull, Hull, UK

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Abstract. The partial-wave Lippmann–Schwinger integral equation is reduced to a system of simultaneous linear equations at negative energies and the negative energy solution is analytically continued to positive energies by means of Padé approximants. This method of solution is suitable for application to interactions which contain both attractive and repulsive regions as well as to purely attractive or purely repulsive potentials.

1. Introduction

The off-shell partial-wave T matrix $T_l(p_1, p_2; k^2)$ satisfies the Lippmann–Schwinger equation

$$T_l(p_1, p_2; k^2) = V_l(p_1, p_2) + \int_0^\infty \frac{V_l(p_1, q) T_l(q, p_2; k^2)}{k^2 - q^2 + i\epsilon} \, dq \tag{1.1}$$

at energy k^2. On the energy shell the solution of this equation is (Warburton and Stern 1969)

$$T_l(k, k; k^2) = -\frac{2k}{\pi} \exp(i\delta_l) \sin \delta_l \tag{1.2}$$

where δ_l is the phase shift with orbital angular momentum l. The two-particle interaction V_l vanishes when one of its momentum variables is infinite.

The most convenient form of the two-body T matrix to use in the three-particle equations of Faddeev (1961) is an eigenfunction expansion separable in the off-shell momenta (Lovelace 1964, Bierter and Dietrich 1967a, 1967b, Fuda 1969, Karchenko *et al* 1970). However, such an expansion may be very difficult to evaluate when the potential contains both attractive and repulsive regions (Warburton and Stern 1969, Stern 1969, pp 113–29). This paper describes a simple method of solving equation (1.1) which is applicable to interactions that change sign as well as to purely attractive or purely repulsive interactions. The procedure reduces the integral equation to a system of simultaneous linear equations at negative energies and analytically continues the negative energy solution to positive energies through the upper half k^2 plane by means of Padé approximants. This approach avoids the problems associated with singular integrals at positive energies (Mongan 1969).

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

2. Negative energy solution

At negative definite energies we substitute the transformation

$$q = \frac{x}{1-x} \tag{2.1}$$

which maps the interval $0 \leqslant q \leqslant \infty$ on to the interval $0 \leqslant x \leqslant 1$, into equation (1.1) to obtain

$$T_l(p_1, p_2; k^2) = V_l(p_1, p_2) + \int_0^1 \frac{V_l(p_1; q) T_l(q, p_2; k^2)}{(k^2 - q^2)(1-x)^2} \mathrm{d}x \tag{2.2}$$

in which $V_l = 0$ when the 'x' corresponding to one of its off-shell momenta equals unity. The first step towards establishing a numerical solution of this negative energy integral equation is to replace the integral on the right hand side by a quadrature formula. If Simpson's rule is chosen we obtain

$$T_l(p_1, p_2; k^2) = V_l(p_1, p_2) + \frac{h}{3} \sum_{m=0}^{2n} \frac{c_m V_l(p_1, q_m) T_l(q_m, p_2; k^2)}{(k^2 - q_m^2)(1-x_m)^2} \tag{2.3}$$

where

$$\begin{aligned} &h = x_m - x_{m-1} = \frac{1}{2n} \qquad q_m = \frac{x_m}{1-x_m} \qquad c_0 = c_{2n} = 1 \\ &c_1 = c_3 = \ldots = c_{2n-1} = 4 \qquad c_2 = c_4 = \ldots = c_{2n-2} = 2. \end{aligned} \tag{2.4}$$

If the off-shell momentum variable p_1 is restricted to the mesh points of the numerical integration, equation (2.3) yields a system of $(2n+1)$ simultaneous linear equations

$$\sum_{m=0}^{2n} \left(\delta_{tm} - \frac{h}{3} \frac{c_m V_l(q_t, q_m)}{(k^2 - q_m^2)(1-x_m)^2} \right) T_l(q_m, p; k^2) = V_l(q_t, p) \tag{2.5}$$

where $t = 0, 1, 2, \ldots, 2n$ ($\delta_{mm} = 1, \delta_{tm} = 0$ for $t \neq m$). But, as the potential V_l vanishes when either $m = 2n$ or $t = 2n$, we are in fact left with a system of $2n$ simultaneous linear equations for the partial wave amplitude at negative definite energies k^2

$$\sum_{m=0}^{2n-1} \left(\delta_{tm} - \frac{h}{3} \frac{c_m V_l(q_t, q_m)}{(k^2 - q_m^2)(1-x_m)^2} \right) T_l(q_m, p; k^2) = V_l(q_t, p) \tag{2.6}$$

where $t = 0, 1, 2, \ldots, 2n-1$. This system can be solved very rapidly on a computer to yield $T_l(q_m, p; k^2)$ for $m = 0, 1, 2, \ldots, 2n-1$. (A system of order 40 can be dealt with in a matter of seconds on an ICL 1905E computer.) The rate of convergence to an acceptable solution can be examined by solving equations (2.6) for various orders of the system. However, care should be taken to avoid loss of accuracy due to rounding errors when the number of equations is very large. (It should be remembered that the solution of these equations also yields the values of $T_l(p, q_m; k^2)$ because of time-reversal invariance of the T matrix.) Computer calculations have shown that this system of equations preserves bound state poles of the partial-wave T matrix if the interaction under consideration forms any bound states.

The system of algebraic equations (2.6), when considered as a negative energy representation of the partial-wave Lippmann–Schwinger equation (1.1), is analogous to a negative energy finite difference solution of the partial-wave Schrödinger equation

derived by Stern and Warburton (1972). Simpson's rule was chosen to represent the integral in equation (2.2) because it is a fast reliable method in which the number of mesh points can be varied very easily.

3. Use of Padé approximants

As the scattering amplitude is an analytic function (apart from possible poles on the negative real axis) in the k^2 plane cut along the positive real axis and as it has the well known asymptotic behaviour (Weinberg 1963, Warburton and Stern 1969)

$$T_l(p_1, p_2; k^2) \sim V_l(p_1, p_2) \tag{3.1}$$

at high energies, it can be represented at both positive and negative energies by an $[N, N]$ Padé approximant (Baker 1965, Garibotti and Villani 1969, Caser *et al* 1969)

$$T_l(p_1, p_2; k^2) \simeq \frac{P_N(K)}{Q_N(K)} = \frac{\Sigma_{t=0}^{N} a_t K^t}{\Sigma_{t=0}^{N} b_t K^t} \qquad (K = ik) \tag{3.2}$$

in which it is expected that $a_N/b_N \simeq V_l(p_1, p_2)$. The polynomial coefficients are, of course, functions of p_1 and p_2. The zeros of the denominator polynomial determine whether there are any bound state or resonance poles. If the T matrix is known at $(2N+1)$ negative energy values for a given pair of off-shell momenta, the curve passing through these points can be fitted by means of the approximant (3.2) by using the method described by Stern and Warburton (1972). After the coefficients a_t and b_t $(t = 0, 1, 2, \ldots, N)$ have been computed this Padé approximant can be employed to analytically continue the partial-wave amplitude (for the same pair of off-shell momenta) from negative energies to positive energies through the upper half k^2 plane because such approximants preserve analytic properties of functions such as poles, zeros, and cuts. When $p_1 = p_2$ the analytic continuation can be used to evaluate the partial-wave T matrix on the energy shell, and by comparing the result obtained with that calculated from equation (1.2) one can estimate the order of accuracy of the off-shell amplitude computed from equations (2.6) and (3.2).

It should be noted that the Padé approximant can be used at zero energy whilst equations (2.6) are restricted to $k^2 < 0$.

4. Applications of the method

Computer calculations have been performed with interactions of the form

$$V_l(p_1, p_2) = \sum_{t=1}^{M} \frac{A_t}{\pi} Q_l\left(\frac{p_1^2 + p_2^2 + \mu_t^2}{2p_1 p_2}\right) \tag{4.1}$$

where $Q_l(\ldots)$ is a Legendre function of order l of the second kind. In the coordinate representation this potential has the more familiar form

$$V(r) = \sum_{t=1}^{M} A_t \frac{\exp(-\mu_t r)}{r}. \tag{4.2}$$

The method of solving the integral equation (1.1) described in the preceding sections was first tested on the attractive Yukawa potential $V(r) = -\exp(-r)/r$ for which results

are available from the eigenfunction expansion method (Warburton and Stern 1969, Stern 1969, pp 76–103). Equations (2.6), used with order 40 (ie $h = 0{\cdot}025$), yielded results for the S wave T matrix which were in good agreement with those computed from the first three terms in the eigenfunction expansions at negative energies. The results were obtained more rapidly from the linear equations than from the eigenfunction expansions because evaluation of the coefficients required in each term of the latter involved complicated calculations. Special attention was given to $T_0(p, p; k^2)$ for $p = 0{\cdot}6$, $1{\cdot}0$, and $1{\cdot}5$ (which coincided with three of the mesh points in the numerical integration); between 15 and 21 negative energy values of this amplitude, which were fitted by means of the Padé approximant (3.2), were obtained from equations (2.6) for each value of p. When the three approximants were used for analytic continuations on to the energy shell the results obtained were in excellent agreement with those determined from the S wave phase shifts via equation (1.2).

The reliability of equations (2.6) and (3.2) was also tested on the neutron–proton triplet S state potential (Coester and Yen 1963)

$$V(r) = \frac{4A \exp(-2\mu r)}{r} - \frac{A \exp(-\mu r)}{r} \tag{4.3}$$

with $A = 42{\cdot}48$ and $\mu = 2{\cdot}307$ (Warburton 1966). This interaction has a repulsive core and an attractive outer region. With the values of A and μ just quoted, $k^2 = 1$ represents an energy of 41·5 MeV in the centre of mass frame. Equations (2.6), solved with order 40 over a range of negative energies, and the resulting Padé approximant fits of order [8, 8] to [10, 10] for the cases $p_1 = p_2 = (0{\cdot}6, 1{\cdot}0, 1{\cdot}5)$ preserved the deuteron bound state pole of the off-shell amplitude at $k^2 = -0{\cdot}0535$ (2·22 MeV). When $T_0(p, p; k^2)$, for $p = (0{\cdot}6, 1{\cdot}0, 1{\cdot}5)$, was evaluated on the energy shell by using the relevant approximant the results obtained were in good agreement with those deduced from experimental triplet S state phase shifts via equation (1.2) (Warburton, private communication). When attempts were made with eigenfunction expansions to compute the off-shell neutron–proton amplitude, difficulties were encountered with some of the terms in the series (Stern 1969, pp 113–29). Equations (2.6) and (3.2) appear to be easier to use than eigenfunction expansions for the purpose of solving the partial-wave Lippmann–Schwinger equation numerically for interactions that change sign, such as (4.3).

Calculations have also been successfully carried out with other potentials of the form (4.2), including a nucleon–nucleon singlet S state potential that was studied in another paper (Stern and Warburton 1972).

5. Conclusions

The numerical methods developed in §§ 2 and 3 are suitable for solving the off-shell partial-wave Lippmann–Schwinger equation with interactions which contain both attractive and repulsive regions as well as with purely attractive or purely repulsive potentials. The approach is strongly recommended for those local interactions, such as (4.3), which are difficult to handle effectively with the eigenfunction expansion method. The off-shell scattering amplitude can be computed far more easily by employing the techniques described in this paper than by using the numerical methods of Mongan (1969) which involve the inversion of large complex matrices.

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References

Baker G A 1965 *Adv. theor. Phys.* **1** 1–58
Bierter W and Dietrich K 1967a *Z. Phys.* **202** 74–88
—— 1967b *Nuovo Cim.* **52A** 1209–21
Caser S, Piquet C and Vermeulen J L 1969 *Nucl. Phys.* **B14** 119–32
Coester F and Yen E 1963 *Nuovo Cim.* **30** 674–6
Faddeev L D 1961 *Sov. Phys.–JETP* **12** 1014–9
Fuda M G 1969 *Phys. Rev.* **186** 1078–85
Garibotti C R and Villani M 1969 *Nuovo Cim.* **63A** 1267–79
Karchenko V F, Petrov N M and Kuzmichev V E 1970 *Phys. Lett.* **32B** 19–22
Lovelace C 1964 *Phys. Rev.* **135** B1225–49
Mongan T R 1969 *Nuovo Cim.* B **63** 539–48
Stern M S 1969 *PhD Thesis* University of Hull
Stern M S and Warburton A E A 1972 *J. Phys.* A: *Gen. Phys.* **5** 112–24
Warburton A E A 1966 *Nuovo Cim.* **41** 360–73
Warburton A E A and Stern M S 1969 *Nuovo Cim.* A **60** 131–59
Weinberg S 1963 *Phys. Rev.* **131** 440–60