The off-shell Born approximation for local potentials

1975 J. Phys. A: Math. Gen. 8 1060

(http://iopscience.iop.org/0305-4470/8/7/008)

J. Phys. A: Math. Gen., Vol. 8, No. 7, 1975. Printed in Great Britain.

The off-shell Born approximation for local potentials

A E A Warburton

Department of Applied Mathematics, The University, Hull HU6 7RX, UK

Received 6 December 1974, in final form 24 February 1975

Abstract. Assuming the existence of a (possibly energy-dependent) local potential satisfying $\int_0^\infty |V(r)|r^2\,dr < \infty$, the off-shell partial-wave amplitudes in the Born approximation, $V_l(p_1, p_2)$, are expressed explicitly in terms of the on-shell $V_l(k, k)$ provided that $p_1 + p_2 \leqslant 2k$. A method is suggested for extending the results to $p_1 + p_2 > 2k$.

1. Introduction

To use the Faddeev equations for the study of three-particle interactions at low energies it is necessary to know the two-body scattering amplitudes off the energy shell. These are not uniquely specified by the on-shell amplitudes, which can be measured experimentally, unless some assumption is made about the nature of the two-body interactions. The most reasonable assumption is that these interactions should be described by short-range local potentials, possibly energy-dependent.

The off-shell amplitude is determined by the Lippmann–Schwinger equation which does not involve the potential function $V(r)$ directly but only via the off-shell Born approximation $V_l(p_1, p_2)$ defined by (1.1). Because of the existence of $V(r)$, however, the latter functions are not independent, and the purpose of this paper is to give an explicit procedure to determine them from the on-shell Born approximation $V_l(k, k)$, $l = 0, 1, 2, \ldots$, at a given energy k^2, so that the $V_l(k, k)$ parametrize the potential.

The notation we use is the following: for the potential $V(r)$ the off-shell Born approximation is

$$V_l(p_1, p_2) = -\int_0^\infty \mathrm{j}_l(p_1 r)\,\mathrm{j}_l(p_2 r)\; V(r) r^2\,dr \tag{1.1}$$

so that the scattering amplitude in the Born approximation is

$$f^{\mathrm{B}}(p_1^2 + p_2^2 - 2p_1 p_2 \cos\theta) = \sum_{l=0}^{\infty} (2l+1) V_l(p_1, p_2) \mathrm{P}_l(\cos\theta). \tag{1.2}$$

On-shell, with $p_1 = p_2 = k$,

$$V_l(k, k) = \delta_l^{\mathrm{B}}(k)/k \tag{1.3}$$

where $\delta_l^{\mathrm{B}}(k)$ is the Born approximation to the lth phase shift. If we suppose the $V_l(k, k)$ to be given for $l = 0, 1, 2, \ldots$, then by taking (1.2) with $p_1 = p_2 = k$ we see that $f^{\mathrm{B}}(K^2)$

is given for $0 \leqslant K^2 \leqslant 4k^2$. Inverting (1.2) to obtain

$$V_l(p_1, p_2) = \tfrac{1}{2}\int_{-1}^{1} f^{\mathrm{B}}(p_1^2+p_2^2-2p_1p_2\mu)\mathrm{P}_l(\mu)\,\mathrm{d}\mu, \tag{1.4}$$

we see that $V_l(p_1, p_2)$ is known in principle provided that

$$p_1+p_2 \leqslant 2k. \tag{1.5}$$

Explicit expressions giving $V_l(p_1, p_2)$ in terms of the $V_l(k, k)$ are derived in §§ 2 and 3 and we shall see later in this section that a sufficient condition for their validity, subject to (1.5), is that

$$\int_0^\infty |V(r)|r^2\,\mathrm{d}r < \infty. \tag{1.6}$$

Since

$$f^{\mathrm{B}}(K^2) = -K^{-1}\int_0^\infty \sin Kr\, V(r) r\,\mathrm{d}r \tag{1.7}$$

we see that if $V(r)$ never changes sign then (1.6) is just the condition that the Born approximation to the scattering amplitude should exist in the forward direction, $\theta = 0$.

To consider the region $p_1+p_2 > 2k$ we must restrict the potential further to 'short-range' potentials. By this we mean that there exists $\alpha > 0$ such that

$$\lim_{r\to\infty} \exp(\alpha r)V(r) = 0. \tag{1.8}$$

For such potentials we see from (1.7) that $f^{\mathrm{B}}(K^2)$ is an analytic function in the region given by $-\alpha < \mathrm{Im}\, K < \alpha$ which includes the positive real K^2 axis. Hence $f^{\mathrm{B}}(K^2)$ is uniquely determined for all $K^2 > 0$ by analytic continuation from the region $0^+ \leqslant K^2 \leqslant 4k^2$, which then determines the $V_l(p_1, p_2)$ by (1.4).

Without condition (1.8) $f^{\mathrm{B}}(K^2)$ is not uniquely specified for $K^2 > 4k^2$ so that $V_l(p_1, p_2)$ is indeterminate for $p_1+p_2 > 2k$. It may be noted that Newton's solution to the inverse scattering problem (Newton 1962) exploits this indeterminacy in constructing an infinite number of potentials, each of which gives the correct phase shifts at a given energy. None of these potentials is short-range in the above sense and all give a scattering amplitude singular at $K^2 = 4k^2$.

The method of analytic continuation to be used is a matter of personal preference. In § 4 we suggest a method based on Padé approximants which extends the region of convergence of the series derived in § 2 and gives high accuracy when tested on the Yukawa potential.

The equation we use to calculate the off-shell amplitudes is an extension of a result derived in an earlier paper (Warburton 1972, hereafter referred to as I), where relations between the on-shell Born approximations at different energies and angular momenta were derived on the assumption of the existence of an energy-independent local potential. Those results in I relevant to the present problem are recalled in § 2 but re-expressed so as to be applicable to energy-dependent potentials if necessary. For such an energy-dependent potential $V_l(q, q)$ no longer necessarily equals $\delta_l^{\mathrm{B}}(q)/q$ for $q \neq k$ so that each energy k^2 has to be considered separately, the off-shell amplitude $V_l(p_1, p_2)$ thus being a function also of k.

Rigorous mathematical justification of the results in § 2 has been given in I and is omitted here. As we shall see, the condition for the validity of § 3 is the same as that

for § 2 so that both sections merely require that the potential should satisfy (1.6). For the method of § 4 to be applicable we should need also condition (1.8) as discussed above.

The results may be extended for suitably large l to potentials singular at $r = 0$. We need only consider potentials vanishing identically for $r > \alpha > 0$, since other potentials may be expressed as the sum of such a potential and another potential satisfying (1.6), and the results are linear in the potential. If

$$|V(r)| \leqslant Ar^{-n} \qquad (0 < r \leqslant \alpha, n \geqslant 3) \tag{1.9}$$

then we can derive the results by use of the bound

$$|\mathrm{j}_l(pr)| \leqslant (pr)^l/1.3.5 \ldots (2l+1). \tag{1.10}$$

From (1.1) we see that the $V_l(p_1, p_2)$ exist provided that

$$l > l_0 = [\tfrac{1}{2}(n-3)] \tag{1.11}$$

and we can define a reduced Born scattering amplitude

$$(f^{\mathrm{B}}(K^2))^{\mathrm{red}} = -K^{-1}\int_0^{\alpha}\left(\sin Kr - \sum_{l=0}^{l_0}(-1)^l(Kr)^{2l+1}/(2l+1)!\right)V(r)r\,\mathrm{d}r. \tag{1.12}$$

With

$$K^2 = p_1^2 + p_2^2 - 2p_1p_2\cos\theta$$

it is easy to see, by using the identity

$$\sin Kr/Kr = \sum_{l=0}^{\infty}(2l+1)\mathrm{j}_l(p_1r)\mathrm{j}_l(p_2r)\mathrm{P}_l(\cos\theta), \tag{1.13}$$

that the right-hand side of (1.12) differs from

$$\sum_{l=l_0+1}^{\infty}(2l+1)V_l(p_1, p_2)\mathrm{P}_l(\cos\theta)$$

only by a polynomial in $\cos\theta$ of degree l_0. Hence the arguments of §§ 2 and 3 may be applied to $(f^{\mathrm{B}})^{\mathrm{red}}$ provided that $l > l_0$.

2. The on-shell amplitude

As discussed in § 1, knowledge of $V_l(k, k)$ for all l and any k implies knowledge of $V_m(q, q)$ for all m and any q in $[0, k]$. For an energy-independent potential this equals $\delta_l^{\mathrm{B}}(q)/q$, the on-shell amplitude. Explicitly, if we set

$$\mu' = 1-(1-\mu)q^2/k^2 \tag{2.1}$$

then

$$\sum_{l=0}^{\infty}(2l+1)V_l(q, q)\mathrm{P}_l(\mu)$$
$$= f^{\mathrm{B}}(2q^2(1-\mu)) = f^{\mathrm{B}}(2k^2(1-\mu')) = \sum_{m=0}^{\infty}(2m+1)V_m(k, k)\mathrm{P}_m(\mu'). \tag{2.2}$$

Hence

$$V_l(q,q) = \sum_{m=l}^{\infty} R_{lm}(q^2/k^2)V_m(k,k) \tag{2.3}$$

where

$$R_{lm}(\alpha) = \tfrac{1}{2}(2m+1)\int_{-1}^{1} P_l(\mu)P_m(1-\alpha+\alpha\mu)\,d\mu \tag{2.4}$$

$$= (2m+1)(m+l+1)^{-1}\alpha^l P_{m-l}^{(2l+1,\,-1)}(1-2\alpha) \tag{2.5}$$

(the R_{lm} vanish identically for $m < l$). The properties of the R_{lm} may be deduced from those of the Jacobi polynomials (Szegö 1939). $R_{lm}(\alpha)$ is a polynomial in α of degree m with an l-fold zero at $\alpha = 0$ and also vanishing at $\alpha = 1$ unless $m = l$ (as can be seen by setting $q = k$ in (2.3)). They are easily generated via the recurrence relation, valid for $m \geqslant l+2$,

$$\begin{aligned}(m-l)(m+l+1)(m-1)(2m+1)^{-1}R_{l,m}(\alpha) &= [m(m-1)(1-2\alpha)+l(l+1)]R_{l,m-1}(\alpha) \\ &\quad -m(m+l-1)(m-l-2)(2m-3)^{-1}R_{l,m-2}(\alpha)\end{aligned} \tag{2.6}$$

starting from

$$\begin{aligned}R_{l,l}(\alpha) &= \alpha^l \\ R_{l,l+1}(\alpha) &= (2l+3)\alpha^l(1-\alpha).\end{aligned} \tag{2.7}$$

The condition $0 < q < k$ implies $0 < \alpha < 1$ where the Jacobi polynomials, and hence the R_{lm}, fall off as $m^{-1/2}$ as $m \to \infty$. Convergence of (2.3) is thus rapid for short-range potentials, as is shown numerically for a typical case in table 1 where we use $\alpha = \frac{1}{2}$ and find accuracy to four decimal places after seven terms of the series.

Table 1. Values of $\Sigma_{m=l}^{M} R_{lm}(\frac{1}{2})V_m(1,1)$ for $V(r) = -e^{-r}/r$.

M	$l=0$	$l=1$	$l=2$	$l=3$
0	0·4024	—	—	—
1	0·5577	0·0518	—	—
3	0·5485	0·1006	0·0171	0·0013
5	0·5494	0·0984	0·0215	0·0046
7	0·5493	0·0986	0·0212	0·0049

This rate of convergence is found to be typical for short-range potentials but the convergence is slower in the following cases:

(i) Large k^2. Here the $V_m(k,k)$ fall off more slowly as $m \to \infty$. Each term of (2.3), and hence the sum to N terms, tends to zero as $k^2 \to \infty$, yet the sum $V_l(q,q)$ is independent of k^2.

(ii) Long-range potentials, for the same reason, since by re-scaling the Schrödinger equation the range can be reduced at the expense of increasing k^2.

(iii) Small q^2. For small α the $R_{lm}(\alpha)$ fall off more slowly as $m \to \infty$. From (2.4) we see that

$$|R_m(\alpha)| \leqslant 2m+1 \tag{2.8}$$

but this bound is only achieved (for $m \neq l$) if both $\alpha = 0$ (ie $q^2 = 0$) and $l = 0$. In this case we have, from (2.3),

$$V_0(0,0) = \sum_{m=0}^{\infty} (2m+1)V_m(k,k) = f^{\mathrm{B}}(0) \tag{2.9}$$

which will always be the most slowly convergent case. For $l \neq 0$, $V_l(q,q)$ tends to zero as $q \to 0$, as does $R_{lm}(q^2/k^2)$, so that no difficulty arises (for short-range potentials both vanish as q^{2l}). The case $l = 0$ merits closer attention for $\alpha \neq 0$. We may integrate (2.4) explicitly to obtain, for $m \geqslant 1$,

$$R_{0m}(\alpha) = \tfrac{1}{2}\alpha^{-1}(\mathrm{P}_{m-1}(1-2\alpha) - \mathrm{P}_{m+1}(1-2\alpha)) \tag{2.10}$$

whence, using

$$|\mathrm{P}_n(x)| \leqslant (2/\pi n)^{1/2}(1-x^2)^{-1/2},$$

for $m \geqslant 2$

$$|R_{0m}(\alpha)| \leqslant [8\pi(\alpha^3 - \alpha^4)]^{-1/2}[(m-1)^{-1/2} + (m+1)^{-1/2}]. \tag{2.11}$$

This bound reflects the asymptotic behaviour of R_{0m} as $m \to \infty$ and shows how $R_{0m}(\alpha)$ can increase as $\alpha \to 0$ for fixed m, although (2.8) gives a limit to that increase.

3. The off-shell amplitude

If we now set

$$\mu' = 1 - (p_1^2 + p_2^2 - 2p_1p_2\mu)/2q^2 \tag{3.1}$$

with the particular choice

$$q = \tfrac{1}{2}(p_1 + p_2) \tag{3.2}$$

then, proceeding as in § 2 we find

$$V_l(p_1, p_2) = \sum_{m=l}^{\infty} (-1)^{m-l} R_{lm}(p_1p_2/q^2)V_m(q,q) \tag{3.3}$$

since

$$\tfrac{1}{2}(2m+1)\int_{-1}^{1} \mathrm{P}_l(\mu)P_m(-1+\alpha+\alpha\mu)\,\mathrm{d}\mu = (-1)^{m-l}R_{lm}(\alpha) \tag{3.4}$$

where

$$\alpha = p_1p_2/q^2 \leqslant 1. \tag{3.5}$$

(3.3) is the same series as (2.3) apart from the factor $(-1)^{m-l}$. It follows that all questions of convergence of the off-shell series have already been answered by the discussion of the convergence of the on-shell series in I, ie that (3.3) converges provided that (1.6) is satisfied.

We note the following properties of the series (3.3):

(i) Each term behaves as $(p_1p_2)^l$ as either p_1 or $p_2 \to 0$ as is the case for $V_l(p_1, p_2)$ for short-range potentials, by (1.1).

(ii) Only the $V_m(q, q)$ (and hence the $V_m(k, k)$ by (2.3)) for $m \geqslant l$ are required.

In view of the similarity of the series (3.3) and (2.3) there is no need to give numerical examples: the rates of convergence are exactly the same for appropriate values of the parameters. The slowly convergent region of small α corresponds to either p_1 or p_2 being small, in which case $V_l(p_1, p_2)$ will be small, as discussed in (i) above, unless $l = 0$.

To summarize, evaluation of $V_l(p_1, p_2)$ from the $V_m(k, k)$ for $m \geqslant l$ involves two steps. Firstly one uses (2.3) to evaluate the $V_m(q, q)$ for $m \geqslant l$ where $q = \frac{1}{2}(p_1 + p_2)$, and then one uses (3.3) to deduce the $V_l(p_1, p_2)$. Both these steps involve the same functions $R_{lm}(\alpha)$. To combine the steps into a single series would involve more computation, owing to the much greater complexity of the series coefficients.

4. Continuation to higher energies

By the use of (3.3) we can deduce the $V_l(p_1, p_2)$ from the $V_l(q, q)$ for any p_1 and p_2 by a suitable choice of q. If, however, our starting point is the $V_l(k, k)$ for a given value of k then we can only deduce (via (2.3)) the $V_l(q, q)$ for $q \leqslant k$, and hence the $V_l(p_1, p_2)$ for $p_1 + p_2 \leqslant 2k$, by (3.5). If we try to use (2.3) for $q > k$ for potentials only satisfying (1.6), we find that the series in general diverges. This is because as $m \to \infty$ for $\alpha > 1$, the $R_{lm}(\alpha)$ increase as $m^{-1/2} \exp(\gamma m)$ where $\cosh \gamma = 2\alpha - 1$. (Szegö 1939). For short-range potentials, satisfying (1.8), the $V_m(k, k)$ fall off exponentially, giving an extension to the region of convergence as discussed in I. In principle we could repeat the procedure using (2.3) for higher and higher k, but in practice errors build up very rapidly.

Instead we suggest that to continue the analytic function $V_l(q, q)$ to the region $q > k$ one should sum the series (2.3) by means of the generalizations of the Aitken δ^2 process developed by Shanks (1955). In this method one replaces a sequence of partial sums $S_0, S_1, S_2, \ldots$ (tending to a limit T) by the sequence of Padé approximants $T_{00}, T_{11}, T_{22}, \ldots$ defined below. This sequence in general converges in a wider region than the original sequence. In the present case we find numerically that the Padé sequence converges for all $q > k$, although more slowly as $q \to \infty$. Typical results are displayed in table 2.

Table 2. Values of $S_M = \sum_{m=l}^{M} R_{lm}(2{\cdot}5) V_m(1, 1)$ for $V(r) = -e^{-r}/r$, and the sequence of Padé approximants T_{ii}, $i = 0, 1, 2, 3$.

$l = 0$			$l = 1$		
M	S_M	Padé	M	S_M	Padé
0	0·4024	0·4024	1	0·2588	0·2588
2	0·8899	0·2494	3	1·169	0·0899
4	3·947	0·2404	5	7·517	0·0878
6	24·67	0·2398	7	54·07	0·0877

The rate of convergence for $q < k$ is also improved, except near $q = 0$. Of course, any other method of analytic continuation would lead to the same results. The Padé approximants used are the diagonal elements of the Padé table T_{ij}. These are easily calculated iteratively by the so called ϵ algorithm (Wynn 1966).

5. Discussion

From a practical point of view the results we have obtained are most readily applicable for large values of the angular momentum l. As l increases we see from (1.1) that $V_l(p_1, p_2)$ decreases so that the Born approximation becomes a better and better approximation to the partial-wave amplitude, both on and off the energy shell. We can thus suppose that the $V_l(k, k)$ are known experimentally for $l \geqslant M$, say. As (2.3) and (3.3) only involve $m \geqslant l$ it follows that the $V_l(p_1, p_2)$ for $l \geqslant M$ can be deduced immediately and be taken as good approximations to the off-shell partial-wave amplitude. Even taking $M = 1$ is likely to give a better approximation to these amplitudes than neglecting them entirely, as is often done.

For $l < M$ we can regard the $V_l(k, k)$ as M parameters of the potential, to be determined by the requirement that the solution of the Lippmann–Schwinger equation should yield the correct phase shifts $\delta_0(k), \ldots, \delta_{M-1}(k)$. However, it may be pointed out that, in principle, equation (3.6) of I gives an explicit expression for the $V_l(k, k)$ for $l < M$ in terms of the $V_m(q, q)$ for $m \geqslant M$.

References

Newton R G 1962 *J. Math. Phys.* **3** 75–82
Shanks D 1955 *J. Math. & Phys.* **34** 1–42
Szegö G 1939 *Orthogonal Polynomials* (New York: American Mathematical Society)
Warburton A E A 1972 *Nuovo Cim.* **12B** 72–82
Wynn P 1966 *Numer. Math.* **8** 264