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Approximations to the Newton potential

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Abstract. Explicit expressions are obtained for Newton's solution to the inverse scattering problem in the approximations where up to two phase shifts are treated exactly and the rest to first order.

1. Introduction and discussion

Results of two-particle elastic scattering experiments provide insufficient data for the prediction of three-particle scattering, since in the latter case the two-particle subsystems need not conserve energy. Thus there is practical interest in the inverse scattering problem of constructing potentials which yield a given set of phase shifts. The only practicable scheme is that due to Newton (1962) and Sabatier (1966), who assume knowledge of all the phase shifts at a given energy. The result is a wide class of phase-equivalent potentials, most of them, however, having unattractive features such as oscillating long-range tails, non-analyticity, etc. All have the property of being extremely difficult to calculate, let alone use within another calculation.

The only physically reasonable case for which manageable expressions are available is the original potential of Newton (1962). This has been used by Underhill (1970) to obtain equations for the two-particle off-shell scattering amplitudes which are required by the three-particle theory of Faddeev (1961). Even here the complexity of the calculation is enormous, and there is no guarantee that a realistic potential is being used.

The purpose of this paper is to present simple explicit approximations to the Newton potential. These are easily calculable and are found only to involve errors which are small compared with the likely errors due to using the Newton potential in the first place.

In § 2 we summarize the general theory of the Newton potential. Construction of the potential consists firstly of evaluating the parameters c_l via (2.7) and (2.14). The problem here is to invert the infinite matrix $(1+R)$, the usual suggestion being to set all phase shifts zero beyond a certain point, so that only a finite matrix need be inverted. In § 3, however, it is shown that if δ_0 and δ_1 are treated exactly, and all other phase shifts to first order, then $(1+R)^{-1} = 1 - CR$, where C is a constant. As a result we obtain explicit expressions for the c_l. The second step in the calculation of the potential is the solution of the system (2.1). In principle this involves inverting large matrices, but within the above approximation one can solve for ϕ_0 and ϕ_1, and essentially use the Born approximation for the remaining ϕ_l. This is described in § 4. The potential is finally deduced from (2.5).

In § 5 numerical results are presented for the Newton potential constructed from the phase shifts of Yukawa potentials. We find that the approximations of treating N phase shifts exactly and the rest to first order converge rapidly as N increases. The resulting potential shows overall similarity to the original potential, but differs in detail. (Attempts to improve the agreement by varying the parameter λ of (2.14) were not successful.) The results suggest that the Newton potential is good enough if one is only interested in accuracies of the order of 10%, and that in this case the approximations presented here only add a negligible error. However, off-shell calculations would not necessarily suffer from so great an inaccuracy, since the amplitudes will be correct on-shell, and only gradually lose accuracy as one extrapolates off-shell.

The Firsov procedure (Vollmer 1969) for constructing approximate potentials requires as input data the phase shifts for non-integer l. An *ad hoc* interpolation is required, which will only be reliable when there is a large number of significant phase shifts, i.e. for long-range interactions. Thus the method is not appropriate where short-range forces dominate, as in most Faddeev calculations.

2. The Newton potential

We summarize here the results of Newton (1962) and Sabatier (1966). If $\phi_l(k, r)$, $l = 0, 1, 2, \ldots$, satisfy the equations

$$\phi_l(k,r) = u_l(kr) - \sum_{m=0}^{\infty} L_{lm}(kr) c_m \phi_m(k,r) \tag{2.1}$$

where

$$u_l(z) = z j_l(z) \tag{2.2}$$

and

$$L_{lm}(z) = \int_0^z j_l(y) j_m(y)\, \mathrm{d}y \tag{2.3}$$

$$= [u_m(z)u_l'(z) - u_l(z)u_m'(z)]/(l-m)(l+m+1), \qquad (m \neq l), \tag{2.4}$$

then the $\phi_l(k, r)$ satisfy the Schrödinger equation for the potential

$$V(r) = -2(kr)^{-1} \frac{\mathrm{d}}{\mathrm{d}r}(r^{-1}K(r)) \tag{2.5}$$

where

$$K(r) = \sum_{m=0}^{\infty} c_m \phi_m(k,r) u_m(kr). \tag{2.6}$$

By letting $r \to \infty$ we can find conditions on the constants c_l in order that a given set of phase shifts $\delta_l(k)$ be obtained from the potential (2.5). These are that

$$c_l^{-1} = -\tfrac{1}{2}\pi/(2l+1) + \left(1 - \sum_{m=0}^{\infty} M_{lm} \tan \delta_m a_m\right) a_l^{-1} \tag{2.7}$$

where the constants a_l satisfy the equations

$$\sum_{m=0}^{\infty} M_{lm}a_m + \sum_{m=0}^{\infty} \tan\delta_l M_{lm} \tan\delta_m a_m = \tan\delta_l, \tag{2.8}$$

and

$$M_{lm} = \begin{cases} [(m-l)(m+l+1)]^{-1}, & (m-l)\text{ odd} \\ 0, & (m-l)\text{ even.} \end{cases} \tag{2.9}$$

Sabatier has constructed the vector $\boldsymbol{v}$, unique to within a constant factor, such that $M\boldsymbol{v}=0$, together with a matrix M^{-1} such that $(MM^{-1})=(M^{-1}M)=I$. Explicitly

$$v_{2l+1}=0,$$

$$v_{2l}=(4l+1)16^{-l}\left[\binom{2l}{l}\right]^2, \tag{2.10}$$

$$M^{-1}_{lm}=0, \qquad (l-m)\text{ even}$$

and

$$M^{-1}_{2l,2m+1} = -M^{-1}_{2m+1,2l} = T_{lm}v_{2l}v_{2m} \tag{2.11}$$

where

$$T_{lm}=(4m+3)(2m+1)^2/(4m+1)(2l-2m-1)(2l+2m+2). \tag{2.12}$$

In matrix notation, with Δ the diagonal matrix such that $\Delta_{ll}=\tan\delta_l$, and $\boldsymbol{e}$ the column matrix with all elements unity, equation (2.8) reads

$$M\boldsymbol{a}+\Delta M\Delta\boldsymbol{a}=\Delta\boldsymbol{e} \tag{2.13}$$

the general solution to which is

$$\boldsymbol{a}=(1+R)^{-1}M^{-1}\Delta\boldsymbol{e}+\lambda(1+R)^{-1}\boldsymbol{v} \tag{2.14}$$

where

$$R=M^{-1}\Delta M\Delta \tag{2.15}$$

and λ is an arbitrary constant. Sabatier has shown that $V(r)$ will have an oscillating tail falling off as $r^{-3/2}$ unless

$$\lim_{l\to\infty}(a_{2l}-a_{2l+1})=0. \tag{2.16}$$

This condition requires that

$$\lambda=\boldsymbol{v}^T\Delta(\boldsymbol{e}-M\Delta\boldsymbol{a}). \tag{2.17}$$

Note that (2.17) involves a_i only for i odd, for which values (2.14) does not involve λ, since $R_{lm}=0$ unless $(l-m)$ is even. Thus λ is given explicitly, and the problem of constructing the Newton potential consists essentially of inverting the matrix $(1+R)$ and solving the equations (2.1).

3. The potential parameters

In this section we calculate the coefficients c_l of the Newton potential in the approximations where N ($=0$, 1 or 2) phase shifts are treated exactly, and the rest to first order.

3.1. N=0

We consider all the phase shifts to be small, i.e. we work essentially in the Born approximation. By (2.15) R is a second-order small quantity and may be neglected. Thus

$$\boldsymbol{a}^{(0)}=M^{-1}\Delta\boldsymbol{e}+\lambda^{(0)}\boldsymbol{v} \tag{3.1}$$

where

$$\lambda^{(0)}=\boldsymbol{v}^T\Delta\boldsymbol{e} \tag{3.2}$$

so that, by (2.7),

$$c_l^{(0)}=[-\tfrac{1}{2}\pi/(2l+1)+1/a_l^{(0)}]^{-1}. \tag{3.3}$$

In each of these equations errors are of third order in the δ_l, thus the equations are in fact correct to second order in the δ_l. (To first order in the δ_l (3.3) simplifies to $c_l^{(0)}=a_l^{(0)}$.)

Explicitly

$$\lambda^{(0)}=\sum_{m=0}^{\infty} v_{2m}\tan\delta_{2m} \tag{3.4}$$

so that

$$a_{2l}^{(0)}=\sum_{m=0}^{\infty} v_{2l}v_{2m}(\tan\delta_{2m}+T_{lm}\tan\delta_{2m+1}) \qquad \text{and} \qquad a_{2l+1}^{(0)}=-\sum_{m=0}^{\infty} v_{2l}v_{2m}T_{ml}\tan\delta_{2m} \tag{3.5}$$

where the constants v_{2l} and T_{lm} are given by (2.10) and (2.12) and do not depend on the phase shifts. The condition (2.16) is satisfied exactly, so that the potential will have no oscillating $r^{-3/2}$ tail.

3.2. N=1

We now treat δ_0 exactly, but all other phase shifts to first order. As $M_{00}=0$, R is a first-order small quantity, so that we can set $(1+R)^{-1}=(1-R)$. In this section all equations will be correct in the above approximation only, although they may contain higher order terms. Thus, for example, we shall set

$$\Delta M\Delta M^{-1}\Delta=\beta_0\Delta \tag{3.6}$$

where

$$\begin{aligned}\beta_0&=\tan\delta_0\sum_{m=0}^{\infty} M_{0,2m+1}\tan\delta_{2m+1}M^{-1}_{2m+1,0}\\&=\tan\delta_0\left(\frac{3}{4}\tan\delta_1+\frac{7}{64}\tan\delta_3+\frac{11}{256}\tan\delta_5+\dots\right)\end{aligned} \tag{3.7}$$

a first-order small quantity.

Using (3.6) and (2.14) we find for the odd a's, to which the term containing λ does not contribute,

$$\boldsymbol{a}_{\text{odd}}^{(1)}=(1-M^{-1}\Delta M\Delta)M^{-1}\Delta\boldsymbol{e}=(1-\beta_0)\boldsymbol{a}_{\text{odd}}^{(0)}. \tag{3.8}$$

Hence (2.17), which only uses the odd a's, gives

$$\lambda^{(1)}=(1-\beta_0)\lambda^{(0)}. \tag{3.9}$$

Returning to (2.14) we thus find

$$\boldsymbol{a}^{(1)}=(1-\beta_0)\boldsymbol{a}^{(0)}-\boldsymbol{\beta}\tan\delta_0 \tag{3.10}$$

using $\lambda^{(0)}=\tan\delta_0+$small terms. Here $\boldsymbol{\beta}=R\boldsymbol{v}$ so that

$$\beta_{2l+1}=0$$

$$\begin{aligned}\beta_{2l}&=\tan\delta_0\sum_{m=0}^{\infty}M^{-1}_{2l,2m+1}\tan\delta_{2m+1}M_{2m+1,0}\\ &=-\tan\delta_0\sum_{m=0}^{\infty}T_{lm}v_{2l}v_{2m}\tan\delta_{2m+1}/(2m+1)(2m+2).\end{aligned} \tag{3.11}$$

Thus treating δ_0 exactly involves only a small modification of the Born approximation. Dropping the second-order terms in (3.10) gives explicitly

$$a^{(1)}_{2l}=a^{(0)}_{2l}+\tan^2\delta_0\sum_{m=0}^{\infty}v_{2l}v_{2m}\tan\delta_{2m+1}(T_{lm}+T_{0m})/(2m+1)(2m+2)$$

and

$$a^{(1)}_{2l+1}=a^{(0)}_{2l+1}-\tan^2\delta_0\sum_{m=0}^{\infty}v_{2l}v_{2m}\tan\delta_{2m+1}T_{0l}T_{0m}/(2m+1)(2m+2). \tag{3.12}$$

Both (3.10) and (3.12) satisfy the condition (2.16).

3.3. $N=2$

If both δ_0 and δ_1 are treated exactly, then R is no longer considered small, but we can still invert $(1+R)$ explicitly to first order in the remaining δ_l. The reason is that, correct to this approximation,

$$R^2=(\beta_0+\epsilon_0)R \tag{3.13}$$

where β_0 is given by (3.7), but is no longer small, while

$$\begin{aligned}\epsilon_0&=\tan\delta_1\sum_{k=1}^{\infty}M_{1,2k}\tan\delta_{2k}M^{-1}_{2k,1}\\ &=\tan\delta_1\left(\frac{15}{64}\tan\delta_2+\frac{3}{256}\tan\delta_4+\ldots\right).\end{aligned} \tag{3.14}$$

The derivation of (3.13) is straightforward but tedious. It follows from (3.13) that, to the same approximation,

$$(1+R)^{-1}=1-(1+\beta_0+\epsilon_0)^{-1}R. \tag{3.15}$$

For computational purposes it is most convenient to use (3.15) as it stands, although this leads to a violation of (2.16) of second order in the small phase shifts. Alternatively, the second-order terms can be dropped on substituting (3.15) into (2.14), when $\boldsymbol{a}^{(2)}$ and $\lambda^{(2)}$

are found to be explicit summations over the small phase shifts, the coefficients in the summations not involving further summations. For example

$$\lambda^{(2)} = (1+\alpha)^{-1} \tan \delta_0 + \sum_{m=2}^{\infty} \lambda_m^{(2)} \tan \delta_m$$

where $\alpha = \frac{3}{4} \tan \delta_0 \tan \delta_1$,

$$\lambda_{2m+1}^{(2)} = -(1+\alpha)^{-2} \tan^2 \delta_0 M_{0,2m+1} M_{2m+1,0}^{-1} \tag{3.16}$$

$$\lambda_{2m}^{(2)} = \left(1 - \frac{2\alpha M_{2m,1}}{1+\alpha}\right)\left(v_{2m} - \frac{2\alpha M_{1,2m}^{-1}}{3(1+\alpha)}\right).$$

It is straightforward to derive similar expressions for $\boldsymbol{a}^{(2)}$.

4. The approximate potentials

Having calculated the c_l to the desired accuracy, we must now solve (2.1) to the same accuracy in order to deduce the corresponding approximation to the Newton potential. To deal with these equations we need a stronger assumption than that the phase shifts be small, which could be fortuitous, but that $\phi_l \approx u_l (l \geqslant N)$ for all r, not just as $r \to \infty$.

For a potential $V(r)$ the Born approximation

$$\delta_l = -k \int_0^{\infty} j_l^2(kr) V(r) r^2 \, \mathrm{d}r \tag{4.1}$$

becomes small either due to (i) $V(r)$ being small, or (ii) $j_l(kr)$ becoming small as $l \to \infty$. In terms of the Newton potential the two cases correspond to (i) the c_l being small ($N = 0$), and (ii) L_{lm} becoming small as l or $m \to \infty$ ($N \neq 0$, when no c_l are small). We see from (2.1) that both cases are dealt with by working to first order in L_{lm} for l or $m \geqslant N$.

If we set

$$S_l = \sum_{m=0}^{\infty} L_{lm} c_m u_m \tag{4.2}$$

then (2.1) can be written

$$\sum_{m=0}^{\infty} (\delta_{lm} + L_{lm} c_m)(\phi_m - u_m) + S_l = 0 \tag{4.3}$$

and (2.6) as

$$K = K_0 - \sum_{m=0}^{\infty} S_m c_m (\phi_m - u_m) \tag{4.4}$$

where

$$K_0 = \sum_{m=0}^{\infty} c_m u_m (u_m - S_m). \tag{4.5}$$

These equations are exact, but working to first order in L_{lm} for l or $m \geqslant N$ we see that $(\phi_l - u_l)$ and S_l are small for $l \geqslant N$, so that equations (4.3), for $l < N$, yield N linear equations for the $(\phi_m - u_m)$ needed in (4.4).

4.1. $N=0$

Here

$$K=K_0=\sum_{m=0} c_m u_m^2+O(\delta_l^2). \tag{4.6}$$

4.2. $N=1$

Here δ_0 is not small and ϕ_0 is given by (4.3) i.e.

$$(1+L_{00}c_0)(\phi_0-u_0)+S_0=0.$$

Thus

$$K=K_0+c_0S_0^2/(1+L_{00}c_0) \tag{4.7}$$

4.3. $N=2$

When δ_0 and δ_1 are both to be treated exactly

$$K=K_0+\frac{[(1+L_{00}c_0)c_1S_1^2+(1+L_{11}c_1)c_0S_0^2-2L_{01}c_0c_1S_0S_1]}{[(1+L_{00}c_0)(1+L_{11}c_1)-L_{01}c_0c_1]}. \tag{4.8}$$

The series in the expressions for S_0, S_1 and K_0 in (4.7) and (4.8) are not, of course, truncated. Numerical differentiation techniques may be used to derive $V(r)$ from $K(r)$ via (2.5).

5. Numerical results

To test the accuracy and validity of the method the input phase shifts were put equal to the phase shifts for the Yukawa potentials $-e^{-r}/5r$ and $-e^{-r}/r$. The resulting approximations to the Newton potential were compared with each other and with the original potential. An energy of $k^2=1$ was used.

The first potential is weak enough for the Born approximation to be accurate to 4% even for $l=0$, and in table 1 we see that the approximations converge very rapidly to the

Table 1. The Newton potential derived from the phase shifts for $V(r)=-e^{-r}/5r$ at $k^2=1$ in the approximation where N ($=0, 1, 2$) phase shifts are treated exactly and the rest to first order, and the approximation where all phase shifts are treated to second order. ($-V(r)$ is shown.) Here $\delta_0=0{\cdot}0834$; $\delta_1=0{\cdot}0210$; $\delta_2=0{\cdot}0064$; etc.

r	Original potential	$N=0$	$N=0$ (2nd order)	$N=1$	$N=2$
0·2	0·8187	0·5728	0·6136	0·6122	0·6128
0·4	0·3352	0·2757	0·2872	0·2869	0·2872
0·6	0·1829	0·1725	0·1745	0·1747	0·1748
0·8	0·1123	0·1182	0·1161	0·1166	0·1167
1·0	0·0736	0·0841	0·0803	0·0808	0·0809
1·5	0·0298	0·0368	0·0332	0·0335	0·0336
2·0	0·0135	0·0148	0·0134	0·0133	0·0135
2·5	0·0066	0·0052	0·0055	0·0053	0·0053
3·0	0·0033	0·0020	0·0029	0·0027	0·0026

Newton potential. The latter is considerably different from the original potential, although of similar overall behaviour. We see that there is little point in going beyond the $N = 0$ case, provided one works to order δ_l^2, i.e. takes c_l from (3.3) rather than setting $c_l = a_l$, and sets $K = K_0$ from (4.5) rather than (4.6).

For the relatively strong attractive potential $V(r) = -e^{-r}/r$, however, we see from table 2 that keeping the second-order terms reduces the accuracy of the $N = 0$ approximation. The $N = 2$ results show that the Newton potential again only bears a superficial resemblance to the original potential.

Table 2. As for table 1 but for $V(r) = -e^{-r}/r$. Here $\delta_0 = 0{\cdot}4800$; $\delta_1 = 0{\cdot}1116$; $\delta_2 = 0{\cdot}0327$; etc.

r	Original potential	$N = 0$	$N = 0$ (2nd order)	$N = 1$	$N = 2$
0·2	4·0937	3·7750	5·7840	5·7154	6·0321
0·4	1·6758	1·8100	1·0307	2·0691	2·1434
0·6	0·9147	1·1244	−0·3624	0·9754	0·9997
0·8	0·5617	0·7628	−0·8266	0·4974	0·5169
1·0	0·3679	0·5349	−0·8824	0·2554	0·2872
1·5	0·1488	0·2199	−0·3602	0·0375	0·1057
2·0	0·0677	0·0774	0·2043	0·0099	0·0561
2·5	0·0328	0·0202	0·4079	0·0239	0·0223
3·0	0·0166	0·0056	0·2975	0·0336	0·0126

It should be emphasized that this difference is not due to a lack of convergence of the approximations, but to the fact that the Newton potential is only one of a wide class of phase-equivalent potentials. This is most clearly seen for very weak potentials, where we can use the Born approximations to the phase shifts as input, and compare the original potential with the $N = 0$ approximation to the Newton potential. We find no better agreement than in table 1.

The Newton potential is thus seen as far from ideal, although it is the best available choice.

References

Faddeev L D 1961 *Sov. Phys.-JETP* **12** 1014–9
Newton R G 1962 *J. Math. Phys.* **3** 75–82
Sabatier P C 1966 *J. Math. Phys.* **7** 1515–31
Underhill J 1970 *J. Math. Phys.* **11** 1409–19
Vollmer G 1969 *Z. Phys.* **226** 424–34