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Complementary bounds on phase shifts

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Abstract. Upper and lower bounds on phase shifts for scattering by short-range potentials are presented. Their derivation is based on complementary variational principles for a certain class of linear operator equations. The well-known Schwinger bound is obtained from this approach together with its complementary bound which appears to be new. The results are illustrated with calculations for a positive step potential.

1. Introduction

In a recent paper (Anderson *et al.* 1970—to be referred to as I) complementary upper and lower bounds were derived on scattering lengths for static potentials. The basic idea was to identify in turn both the differential and integral equations describing zero-energy potential scattering with a general linear equation

$$(Q+T^*T)\phi = f \tag{1}$$

where Q is a symmetric positive-definite operator and T is a linear operator with adjoint T^*. Then complementary variational principles associated with such equations (cf. Arthurs 1969, Robinson 1969) led to the bounds. In the present paper we see that some of the analysis can be extended to the case when the energy is not zero but $\frac{1}{2}k^2$, to yield complementary bounds on phase shifts. For simplicity we restrict ourselves to s-waves, but analogous results with any ℓ quantum number can be obtained.

It seems that for non-zero k only the integral equation for scattering is suitable for the complementary variational principle theory, and as in I we need to assume that the potential is of one sign. One of the bounds obtained is Schwinger's (1947, 1950), but the complementary bound appears to be new. When the phase shift is sufficiently small the bounds are global, but for phases in the second or third quadrants they are local, i.e. third-order terms have to be neglected. Further, in these quadrants we need to work with functionals which are constrained to be stationary with respect to variation in the amplitude of the trial function. Illustrative results are presented for scattering by a positive step potential.

Since phase shifts can now be readily calculated numerically for one-dimensional problems, the interest here is primarily theoretical. However it may prove feasible to extend the ideas to less tractable multi-channel situations. Our methods are different from those of Sugar and Blankenbecler (1964).

2. Preliminary theory

The s-wave $\phi(r)$ can be regarded as the solution of the differential equation

$$\{p(r)-\mathrm{d}^2/\mathrm{d}r^2-k^2\}\phi(r) = 0, \qquad 0 \leqslant r < \infty \tag{2}$$

subject to the conditions

$$\phi(0) = 0 \tag{3}$$

$$\phi(r) \sim A(k)\cos kr - k^{-1}\sin kr \qquad \text{as } r \to \infty. \tag{4}$$

Here

$$p(r) = (2m/\hbar^2)V(r) \tag{5}$$

where $V(r)$ is a short-range potential and m is the mass of the scattered particle. If the phase shift is η, the factor $A(k)$ in (4) is given by

$$A(k) = -k^{-1}\tan\eta = -k^{-1}\int_0^\infty \sin kr\, p(r)\,\phi(r)\,\mathrm{d}r. \tag{6}$$

We have chosen the normalization in (4) and (6) because this leads to bounds for $A(k)$ which, as k tends to zero, go over to those derived in I on the scattering length $A(0)$.

When p is positive we can formally identify equation (2) with equation (1) by taking

$$Q = p, \qquad T = \mathrm{d}/\mathrm{d}r + k\tan kr, \qquad T^* = -\mathrm{d}/\mathrm{d}r + k\tan kr. \tag{7}$$

However, the resulting singularities in T and T^* could destroy the meaning of certain integrals which arise in the theory of the complementary variational principles. Thus the differential equation for scattering does not seem to be directly adaptable to the theory, as it is when $k = 0$. The negative term $(-k^2)$ in the operator spoils things.

It seems then that we should turn to the integral equation for $\phi(r)$, which is

$$\phi(r) + k^{-1}\int_0^\infty \sin(kr_<)\cos(kr_>)p(s)\phi(s)\,\mathrm{d}s = -k^{-1}\sin kr \tag{8}$$

where

$$r_< = \min\{r, s\}, \qquad r_> = \max\{r, s\}. \tag{9}$$

When T and T^* are integral operators on $(0, \infty)$ the complementary bounds associated with equation (1) are (see I)

$$J(\Phi_1) \leqslant I(\phi) \leqslant G(T\Phi_2) \tag{10}$$

where

$$I(\phi) = \int_0^\infty f\phi\,\mathrm{d}r \tag{11}$$

$$J(\Phi_1) = -\int_0^\infty \Phi_1(Q + T^*T)\Phi_1\,\mathrm{d}r + \int_0^\infty 2f\Phi_1\,\mathrm{d}r \tag{12}$$

and

$$G(T\Phi_2) = J(\Phi_2) + \int_0^\infty \{(Q+T^*T)\Phi_2 - f\}Q^{-1}\{(Q+T^*T)\Phi_2 - f\}\,\mathrm{d}r. \tag{13}$$

The trial functions Φ_1 and Φ_2 need satisfy no special conditions, but the nearer they are to the exact solution ϕ the closer the bounds will be to $I(\phi)$.

It is convenient to rewrite equation (8) in the form

$$(p + K)\phi = -k^{-1}\sin kr\, p(r) \tag{14}$$

where K is the symmetric integral operator with kernel

$$k^{-1}p(r)\sin(kr_<)\cos(kr_>)p(s) \tag{15}$$

and to consider the possibility of making the identification

$$\pm(p+K) = Q+T^*T. \tag{16}$$

Then with

$$f = \mp k^{-1}\sin kr\, p(r) \tag{17}$$

we shall have, from (6) and (11),

$$I(\phi) = \pm A(k) = \mp k^{-1}\tan\eta \tag{18}$$

and so from (10) the possibility of bounds on the phase shift.

3. Bounds with positive potentials when $0 > \eta > -\pi/2$

Let us suppose first that p is positive. The symmetric operator K is not positive-definite, but the operator $(p+K)$ may be. As a corollary to Lemma 1, proved in the Appendix, we have the following result:

Lemma 1′. If $p > 0$ and $0 > \eta > -\pi/2$, then $(p+K)$ is positive-definite.

Now choose a positive number γ such that

$$0 < \gamma < 1 \tag{19}$$

and let $\zeta(\gamma)$ be the phase of the s-wave for potential p/γ so that $\eta = \zeta(1)$. Then

$$0 > \eta > \zeta(\gamma) \tag{20}$$

since $\zeta(\gamma)$ is an increasing function of γ when p is positive (see Appendix 1). If we replace p by p/γ in Lemma 1′, we see that the operator $(\gamma^{-1}p+\gamma^{-2}K)$—and therefore also the operator $(\gamma p+K)$—is positive-definite if

$$p > 0, \qquad 0 > \zeta(\gamma) > -\pi/2. \tag{21}$$

Thus if conditions (21) hold, we can set

$$p+K = Q+T^*T \tag{22}$$

where

$$Q = (1-\gamma)p > 0 \tag{23}$$

and

$$T^*T = \gamma p+K. \tag{24}$$

The explicit forms of T and T^* are not required; the operator $(\gamma p+K)$ is symmetric and positive-definite, and as such can be written in the form T^*T for some T and T^* (Mikhlin 1964). We obtain from equations (10)–(13) the bounds

$$A_-(\Phi_1;k) \leqslant A(k) \leqslant A_+(\Phi_2;k) \tag{25}$$

where

$$A_-(\Phi_1;k) = -\int_0^\infty \Phi_1(p+K)\Phi_1\,\mathrm{d}r - \int_0^\infty 2k^{-1}\sin kr\, p(r)\Phi_1\,\mathrm{d}r \tag{26}$$

and

$$A_+(\Phi_2;k) = A_-(\Phi_2;k)+(1-\gamma)^{-1}\int_0^\infty \{(p+K)\Phi_2+k^{-1}\sin kr\, p\}^2 p^{-1}\,\mathrm{d}r. \tag{27}$$

The existence of the bound A_- merely depends on the operator $(p+K)$ being positive-definite. If we consider $A_-(c\Phi_1)$ and maximize with respect to the amplitude c, we recover Schwinger's (1947) bound: see equation (34) below.

The bound A_+ depends on there being a suitable γ for which conditions (19) and (21) hold. It follows from (27) that the most favourable value of γ is zero. This choice is only possible if

$$\lim_{\gamma\to 0} \zeta(\gamma) > -\frac{\pi}{2} \tag{28}$$

a criterion which is not in general easy to test. There will always be some value of γ for which A_+ is a bound if $0 > \eta > -\pi/2$, but it is difficult to determine it in advance.

4. Bounds with negative potentials when $0 < \eta < \pi/2$

There are results similar to those in §3 which hold when p is negative. We have as a corollary to Lemma 2 (see Appendix 2):

Lemma 2′. If $p < 0$ and $0 < \eta < \pi/2$, then $-(p+K)$ is positive-definite. With the same meanings for γ and ζ, it follows that $-(p+K)$ is positive-definite if

$$p < 0, \qquad 0 < \zeta < \pi/2. \tag{29}$$

If these conditions hold we can set

$$-(p+K) = Q+T^*T \tag{30}$$

where

$$Q = -(1-\gamma)p > 0 \tag{31}$$

and

$$T^*T = -(\gamma p+K). \tag{32}$$

This decomposition leads to the complementary bounds

$$-A_-(\Phi_1; k) \leqslant -A(k) \leqslant -A_+(\Phi_2; k) \tag{33}$$

where A_- and A_+ are given by expressions (26) and (27).

5. Bounds when $\pi/2 < |\eta| < \pi$

The amplitude-optimized forms of $A_-(c\Phi_1)$ and $A_+(c\Phi_2)$ (with zero γ) are

$$\tilde{A}_-(\Phi_1) = \frac{\left(\int_0^\infty k^{-1} \sin kr\, p\Phi_1 \,\mathrm{d}r\right)^2}{\int_0^\infty \Phi_1(p+K)\Phi_1 \,\mathrm{d}r} \tag{34}$$

and

$$\tilde{A}_+(\Phi_2) = \int_0^\infty k^{-2} \sin^2 kr\, p \,\mathrm{d}r - \frac{\left(\int_0^\infty k^{-1} \sin kr K\Phi_2 \,\mathrm{d}r\right)^2}{\int_0^\infty K\Phi_2(p^{-1}+K^{-1})K\Phi_2 \,\mathrm{d}r}. \tag{35}$$

It can be proved that if third-order terms in $(\Phi_1-\phi)$ and $(\Phi_2-\phi)$ can be neglected, $\tilde{A}_-$ and $\tilde{A}_+$ provide complementary local bounds on A as follows:

$$\tilde{A}_-(\Phi_1; k) \leqslant A(k) \leqslant \tilde{A}_+(\Phi_2; k) \text{ when } p > 0 \text{ and } -\pi < \eta < -\pi/2 \tag{36}$$

$$-\tilde{A}_-(\Phi_1; k) \leqslant -A(k) \leqslant -\tilde{A}_+(\Phi_2; k) \text{ when } p < 0 \text{ and } \pi > \eta > \pi/2. \tag{37}$$

These results for Schwinger's functional $\tilde{A}_-$ were established by Kato (1951). Expansion of (34) yields

$$\tilde{A}_-(\Phi_1)-A = -\int_0^\infty (\Phi_1-\phi)\Omega(\Phi_1-\phi)\,\mathrm{d}r + r_1(\phi,\Phi_1-\phi)\|\Phi_1-\phi\|^2 \tag{38}$$

where

$$r_1(\phi,\Phi_1-\phi)\to 0 \qquad \text{as } \|\Phi_1-\phi\|\to 0$$

with $\|\ \|$ equal to the usual L_2 norm of real Hilbert space, and where

$$\Omega = p+K-A^{-1}|pk^{-1}\sin kr\rangle\langle pk^{-1}\sin kr| \tag{39}$$

the Dirac notation $|\rangle\langle|$ being used to denote a non-local operator. Kato deduced his results from lemmas equivalent to the following:

Lemma 1. Ω is positive-definite when $p>0$ and $-\pi<\eta<0$
Lemma 2. $-\Omega$ is positive-definite when $p<0$ and $\pi>\eta>0$.

The results for the functional $\tilde{A}_+$ can be established in a similar manner. From (35) we find that

$$\tilde{A}_+(\Phi_2)-A = \int_0^\infty (\Phi_2-\phi)K\Gamma K(\Phi_2-\phi)\,\mathrm{d}r + r_2(\phi,\Phi_2-\phi)\|\Phi_2-\phi\|^2 \tag{40}$$

where

$$r_2(\phi,\Phi_2-\phi)\to 0 \qquad \text{as } \|\Phi_2-\phi\|\to 0$$

and where

$$\Gamma = p^{-1}+K^{-1}-B^{-1}|k^{-1}\sin kr\rangle\langle k^{-1}\sin kr| \tag{41}$$

and

$$B = \int_0^\infty K\phi(p^{-1}+K^{-1})K\phi\,\mathrm{d}r = -A+\int_0^\infty k^{-2}\sin^2 kr\,p\,\mathrm{d}r. \tag{42}$$

In Appendix 3 we prove:

Lemma 3. $K\Gamma K$ is positive-definite when $p>0$ and $-\pi<\eta<-\pi/2$
Lemma 4. $-K\Gamma K$ is positive-definite when $p<0$ and $\pi>\eta>\pi/2$.

The bounding properties of $\tilde{A}_+$ in (36) and (37) now follow from the lemmas and the expansion (40). It should be noted that the functional $\tilde{A}_+$ does not provide bounds when $|\eta|<\pi/2$, except when $|\eta|$ is sufficiently small for A_+ itself to provide bounds as explained in §§ 3 and 4.

6. Summary of results

For convenience we summarize the results at this point.

(i) $p>0$

$$A_-(\Phi_1;k)\leqslant A(k)\leqslant A_+(\Phi_2;k) \qquad -\pi/2<\eta<0 \tag{43}$$

$$\tilde{A}_-(\Phi_1;k)\leqslant A(k) \qquad -\pi<\eta<0 \tag{44}$$

$$A(k)\leqslant \tilde{A}_+(\Phi_2;k) \qquad -\pi<\eta<-\pi/2. \tag{45}$$

(ii) $p<0$

$$-A_-(\Phi_1;k)\leqslant -A(k)\leqslant -A_+(\Phi_2;k) \qquad 0<\eta<\pi/2. \tag{46}$$

$$-\tilde{A}_-(\Phi_1;k)\leqslant -A(k) \qquad 0<\eta<\pi. \tag{47}$$

$$-A(k)\leqslant -\tilde{A}_+(\Phi_2;k) \qquad \pi/2<\eta<\pi. \tag{48}$$

The functionals appearing here are defined in equations (6), (26), (27), (34) and (35).

It should be remembered that in each case $\tilde{A}$ is a special case of A, and also that there are reservations concerning the right-hand inequalities in (43) and (46).

7. An illustration

To illustrate the theory we have calculated the quantities

$$\eta_- = \tan^{-1}(-k\tilde{A}_+) \quad \text{and} \quad \eta_+ = \tan^{-1}(-k\tilde{A}_-) \tag{49}$$

for the case of the step potential

$$\begin{aligned} V = 8 \qquad & 0 \leqslant r \leqslant 1 \\ 0 \qquad & \quad r > 1 \end{aligned} \tag{50}$$

for which the exact phase shift can be determined (Mott and Massey 1965). The scattered particle was chosen to have mass $m = 1$ a.u. and the following simple trial function was used:

$$\Phi = (a \cos kr - k^{-1} \sin kr)(1 - e^{-r}) \tag{51}$$

where a is a variational parameter. This function has the correct behaviour at zero and infinity. Calculations have been performed for a range of values of k and the results are given in table 1 along with the exact values of the phase shift η.

Table 1. Phases η_-, η and η_+ for scattering by potential (50)

k	η_-	η (exact)	η_+ (Schwinger)
0·1	−0·0751	−0·0750	−0·0746
1·5	−1·1172	−1·1160	−1·1080
1·7	−1·2582	−1·2616	−1·2515
2·0	−1·4822	−1·4772	−1·4632
3·0	−2·1713	−2·1569	−2·1077

The quantity η_+ corresponds to the Schwinger functional and is an upper bound to η for all η in $-\pi < \eta < 0$. The complementary quantity η_- is a lower bound for η sufficiently near zero and for $-\pi < \eta < -\pi/2$, as expected from the results of §§ 3–5. For $\eta = -1{\cdot}2616$ (i.e. $-72°$), corresponding to $k = 1{\cdot}7$, we see that η_- fails to be a lower bound. In this region of η the operator $K\Gamma K$ has ceased to be positive-definite. For this example, if $k < \pi/2$ the criterion (28) actually holds (cf. Mott and Massey 1965), which guarantees that η_- is a lower bound when η is in the fourth quadrant.

Appendix 1. The dependence of $\zeta(\gamma)$ on γ

Let $\phi(\gamma)$ be the s-wave for potential p/γ, with phase $\zeta(\gamma)$. If we integrate the identity

$$\phi(\gamma)\frac{d^2}{dr^2}\phi(\gamma+\delta\gamma) - \phi(\gamma+\delta\gamma)\frac{d^2}{dr^2}\phi(\gamma) = \left(\frac{1}{\gamma+\delta\gamma} - \frac{1}{\gamma}\right)p\phi(\gamma+\delta\gamma)\phi(\gamma) \tag{A1}$$

from $r = 0$ to infinity, and make use of boundary conditions analogous to (3) and (4), we obtain in the limit as $\delta\gamma \to 0$ the result

$$\gamma^2 \sec^2\zeta(\gamma)\frac{d\zeta}{d\gamma} = k\int_0^\infty p\{\phi(\gamma)\}^2\, dr. \tag{A2}$$

This shows that $\zeta(\gamma)$ is an increasing function of γ when $p > 0$, and a decreasing one when $p < 0$.

Appendix 2. Lemmas 1 and 2

To prove Lemma 1 it is enough to show that the functional

$$\left(\int_0^\infty \Psi p \Psi \, \mathrm{d}r\right)^{-1} \int_0^\infty \Psi \Omega \Psi \, \mathrm{d}r \tag{A3}$$

cannot take negative values when $p > 0$ and $-\pi < \eta < 0$. Suppose to the contrary that it can, and let $-\omega^2$ be a negative eigenvalue such that

$$\Omega\psi = -\omega^2 p\psi. \tag{A4}$$

The functional (A3) is bounded below and so ω^2, if it exists, will be finite. It follows from (A4) that

$$\begin{aligned} \psi \sim\; & -(1+\omega^2)^{-1} \cos kr \int_0^\infty k^{-1} p \sin kr \, \psi \, \mathrm{d}r \\ & + (1+\omega^2)^{-1} k^{-1} A^{-1} \sin kr \int_0^\infty k^{-1} p \sin kr \, \psi \, \mathrm{d}r \end{aligned} \tag{A5}$$

for large r, and also that

$$\{-\mathrm{d}^2/\mathrm{d}r^2 - k^2 + (1+\omega^2)^{-1} p\}\psi = 0. \tag{A6}$$

From (A6) and (A2), the phase of ψ, i.e. $\zeta(1+\omega^2)$, is greater than η, i.e. $\zeta(1)$. However, from (A5), the phase of ψ is $\eta - n\pi$ ($n = 0, 1, 2, \ldots$), which leads to a contradiction when $-\pi < \eta < 0$. Thus in that situation the functional (A3) cannot take negative values, and so is positive-definite.

Mutatis mutandis, Lemma 2 can be justified for negative p.

For positive p and $-\pi/2 < \eta < 0$, Ω is positive-definite by Lemma 1. Also A is positive in this quadrant. Hence from (39) we see that $p + K$ is positive definite for $p > 0$ and $-\pi/2 < \eta < 0$, which proves Lemma 1′ stated in § 3. Lemma 2′ follows in a similar way from Lemma 2.

Appendix 3. Lemmas 3 and 4

To prove Lemma 3, it is enough to show that the functional

$$\left\{\int_0^\infty (K\theta) p^{-1} (K\theta) \, \mathrm{d}r\right\}^{-1} \int_0^\infty (K\theta) \Gamma (K\theta) \, \mathrm{d}r \tag{A7}$$

cannot take negative values when $p > 0$ and $-\pi > \eta > -\pi/2$. Suppose to the contrary that it can and let $-\nu^2$ be a negative eigenvalue such that

$$\Gamma K\theta = -\nu^2 p^{-1} K\theta. \tag{A8}$$

The functional (A7) is bounded below and so ν^2, if it exists, will be finite. Equation (A8) simplifies to

$$\theta = -(1+\nu^2) p^{-1} K\theta + (Bk)^{-1} \sin kr \int_0^\infty k^{-1} \sin kr K\theta \, \mathrm{d}r. \tag{A9}$$

It follows that, for large r,

$$\theta \sim -\cos kr(1+\nu^2)\int_0^\infty k^{-1}\sin kr\, p\theta\, dr + (Bk)^{-1}\sin kr \int_0^\infty k^{-1}\sin kr K\theta\, dr \quad \text{(A10)}$$

so that the phase of θ is

$$\tan^{-1}\left\{-kB(1+\nu^2)\int_0^\infty k^{-1}\sin kr\, p\theta\, dr\left(\int_0^\infty k^{-1}\sin kr K\theta\, dr\right)^{-1}\right\}. \quad \text{(A11)}$$

If we premultiply (A9) by $k^{-1}\sin kr\, p$ and integrate, we obtain the relation

$$\int_0^\infty k^{-1}\sin kr\, p\theta\, dr = \left\{B^{-1}\int_0^\infty k^{-2}\sin^2 kr\, p\, dr - (1+\nu^2)\right\}\int_0^\infty k^{-1}\sin kr K\theta\, dr. \quad \text{(A12)}$$

From (A12) and (42), expression (A11) for the phase of θ simplifies to

$$\tan^{-1}\left\{(1+\nu^2)^2\tan\eta + k\nu^2(1+\nu^2)\int_0^\infty k^{-2}\sin^2 kr\, p\, dr\right\} \quad \text{(A13)}$$

which is evidently *greater than* η when $p > 0$ and $-\pi > \eta > -\pi/2$ so that $\tan\eta$ is positive. (We assume that ν^2 is small enough so that the phase of θ is in the same quadrant as η. If this is not the case, we can artificially adjust ν^2 in equation (A8) by considering the operator $\alpha\Gamma$ instead of Γ, where α is a small positive constant.)

On the other hand, if we operate on equation (A9) with $(-d^2/dr^2-k^2)$ the $\sin kr$ term is annihilated, and we see that

$$\{-d^2/dr^2-k^2+(1+\nu^2)p\}\theta = 0. \quad \text{(A14)}$$

Thus the phase of θ is $\zeta\{(1+\nu^2)^{-1}\}$, which is *less than* η when $p > 0$. This contradiction establishes Lemma 3, and Lemma 4 can be justified in a similar manner.

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