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1970 J. Phys. A: Gen. Phys. 3 1

(http://iopscience.iop.org/0022-3689/3/1/001)

Upper and lower bounds on scattering lengths

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MS. received 9*th July* 1969

Abstract. Upper and lower bounds on scattering lengths for static potentials are presented. Their derivation is based on complementary variational principles for a certain class of linear operator equations. The well-known bounds of Schwinger and of Spruch and Rosenberg are obtained from this approach together with related complementary bounds, some of which are new. The results are illustrated with calculations for screened Coulomb potentials.

1. Introduction

The s wave $\phi(r)$ of a zero-energy, potential-scattering process can be specified in two equivalent ways. We can either regard $\phi(r)$ as the solution of the differential equation

$$\{-\mathrm{d}^2/\mathrm{d}r^2+p(r)\}\phi(r) = 0, \qquad 0 \leqslant r < \infty \tag{1}$$

subject to the conditions

$$\phi(0) = 0, \qquad \phi(r) \sim A-r, \qquad \text{as } r \to \infty \tag{2}$$

or alternatively think of it as the solution of the integral equation

$$\phi(r) = -r-\int_0^\infty \min(r, r')p(r')\phi(r')\,\mathrm{d}r'. \tag{3}$$

Here

$$p(r) = \frac{2m}{\hbar^2} V(r) \tag{4}$$

where $V(r)$ is a short-range potential and m is the mass of the scattered particle. The scattering length A is given by the relation

$$A = -\int_0^\infty rp(r)\phi(r)\,\mathrm{d}r. \tag{5}$$

The Spruch–Rosenberg (1959) bound for A arises from the differential equation (DE) approach using a Kohn-type variational principle, whilst the Schwinger bound for A is also derived variationally from the integral equation (IE) approach (see e.g. Moiseiwitsch 1966). Recently it has been shown (Arthurs 1968) that two-sided bounds are obtainable from the IE, and preliminary calculations have been reported for positive screened Coulomb potentials (Anderson and Arthurs 1969).

In this paper we exhibit a number of different bounds which are obtainable from the two approaches, for both positive and negative potentials. New bounds are derived from the DE which are complementary to those of Spruch and Rosenberg, and from the IE which are complementary to Schwinger's. With the IE approach, various decompositions of an operator are possible and lead to alternative bounds.

All the results are presented as special cases of the general theory for a non-homogeneous equation. They are illustrated with calculations for both positive and negative screened Coulomb potentials. In conclusion the relative merits of the DE and IE approaches are briefly discussed.

2. General theory

We consider a physical problem which is described by the linear equation

$$(Q+T^*T)\phi = f \qquad 0 \leqslant r < \infty \tag{6}$$

with

$$\phi = \phi_B \qquad \text{on the boundary of } (0, \infty). \tag{7}$$

Here f is a known function of the coordinate r, ϕ_B specifies the behaviour of the exact solution ϕ at zero and infinity, Q is a symmetric positive-definite operator with a left inverse Q_1^{-1}, and T is a linear operator with adjoint T^* defined by the relation

$$\int_0^\infty uT\phi \, dr = \int_0^\infty (T^*u)\phi \, dr + \sigma_T[u\phi]_0^\infty \tag{8}$$

where σ_T is a numerical factor. We assume that all operators and functions used are real. The applications considered in §§ 3 and 4 correspond to:

$$\text{(i)}\ T = \frac{d}{dr}+\tau(r), \qquad T^* = -\frac{d}{dr}+\tau(r), \qquad \sigma_T = 1 \tag{9}$$

where $\tau(r)$ is either zero or a short-range function of r, and

(ii) T = integral operator, T^* = adjoint integral operator, $\sigma_T = 0$. (10)

Complementary variational principles associated with certain boundary value problems have been developed recently (cf. Arthurs 1969, Robinson 1969). For problems described by equations (6) and (7) these principles lead to upper and lower bounds

$$G(T\Phi_2) \leqslant I(\phi) \leqslant J(\Phi_1) \tag{11}$$

for the functional

$$I(\phi) = -\tfrac{1}{2}\int_0^\infty f\phi \, dr + \tfrac{1}{2}\sigma_T[\phi T\phi]_0^\infty. \tag{12}$$

The expressions for the functionals J and G (which are stationary at ϕ) are

$$J(\Phi_1) = \tfrac{1}{2}\int_0^\infty \Phi_1(Q+T^*T)\Phi_1 \, dr - \int_0^\infty f\Phi_1 \, dr - \sigma_T[(\tfrac{1}{2}\Phi_1-\phi_B)T\Phi_1]_0^\infty \tag{13}$$

and

$$G(T\Phi_2) = -\tfrac{1}{2}\int_0^\infty \Phi_2 T^*T\Phi_2 \, dr - \tfrac{1}{2}\int_0^\infty (f-T^*T\Phi_2)Q_1^{-1}(f-T^*T\Phi_2) \, dr$$
$$-\sigma_T[(\tfrac{1}{2}\Phi_2-\phi_B)T\Phi_2]_0^\infty. \tag{14}$$

From these expressions for J and G it can be verified directly that the bounds in equation (11) hold good, provided that the trial function Φ_1 satisfies

$$\sigma_T[(\Phi_1-\phi_B)T(\Phi_1-\phi)]_0^\infty \leqslant 0. \tag{15}$$

3. Differential equation approach

We now apply the theory of section 2 to the zero-energy scattering problem described by the differential equation (1) subject to the boundary conditions (2). Equations (1) and (2) are examples of (6) and (7). It is convenient to treat the cases $p > 0$ and $p < 0$ separately.

3.1. *The case* $p > 0$

We choose

$$T = \frac{\mathrm{d}}{\mathrm{d}r}, \qquad T^* = -\frac{\mathrm{d}}{\mathrm{d}r}, \qquad \sigma_T = 1 \tag{16}$$

$$Q = p, \qquad f = 0 \tag{17}$$

$$\phi_{\mathrm{B}} = 0 \quad \text{at } r = 0, \qquad \phi_{\mathrm{B}} \sim A - r \text{ as } r \to \infty. \tag{18}$$

Then the results of section 2 apply to equations (1) and (2), provided condition (15) is satisfied; the optimum choice for this condition becomes

$$\left[(\Phi_1 - \phi_{\mathrm{B}}) \frac{\mathrm{d}}{\mathrm{d}r} (\Phi_1 - \phi)\right]_0^\infty = 0. \tag{19}$$

We shall satisfy (19) by taking the trial function Φ_1 such that

$$\Phi_1(0) = 0, \qquad \Phi_1 \sim a_1 - r \quad \text{as} \quad r \to \infty \tag{20}$$

where a_1 is a constant. The basic functionals in (12), (13) and (14) then become

$$I(\phi) = \tfrac{1}{2}(R - A)_{R \to \infty} \tag{21}$$

$$J(\Phi_1) = \tfrac{1}{2} \int_0^\infty \Phi_1 \left(p - \frac{\mathrm{d}^2}{\mathrm{d}r^2}\right) \Phi_1 \, \mathrm{d}r + \tfrac{1}{2}(R - 2A + a_1)_{R \to \infty} \tag{22}$$

and

$$G(T\Phi_2) = \tfrac{1}{2} \int_0^\infty \Phi_2 \frac{\mathrm{d}^2}{\mathrm{d}r^2} \Phi_2 \, \mathrm{d}r - \tfrac{1}{2} \int_0^\infty p^{-1} (\Phi_2'')^2 \, \mathrm{d}r - [(\tfrac{1}{2}\Phi_2 - \phi_{\mathrm{B}})\Phi_2']_0^\infty. \tag{23}$$

The boundary term involving R can be subtracted from each functional, and to get a useful bound from G it is necessary to make the trial function Φ_2 satisfy boundary conditions of the form

$$\Phi_2(0) = 0, \qquad \Phi_2 \sim a_2 - r \qquad \text{as} \quad r \to \infty \tag{24}$$

otherwise the lower bound recedes to minus infinity. Then from $G \leqslant I \leqslant J$ we obtain upper and lower bounds for the scattering length A, namely

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

where

$$A_+(\Phi_1) = a_1 + \int_0^\infty \Phi_1 \left(p - \frac{\mathrm{d}^2}{\mathrm{d}r^2}\right) \Phi_1 \, \mathrm{d}r \tag{26}$$

and

$$A_-(\Phi_2) = a_2 + \int_0^\infty p^{-1} \Phi_2'' \left(p - \frac{\mathrm{d}^2}{\mathrm{d}r^2}\right) \Phi_2 \, \mathrm{d}r. \tag{27}$$

The upper bound (26) is the one due to Spruch and Rosenberg (1959), while the lower bound (27) appears to be new.

3.2. *The case* $p < 0$

When p is negative we cannot set $Q = p$ as in § 3.1, because Q is to be positive-definite. We retain the identification

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + p = Q + T^*T \tag{28}$$

but this time we take

$$Q = (\lambda_0 - 1)(-p) \tag{29}$$

$$T^*T = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \lambda_0 p \tag{30}$$

where λ_0 is the lowest eigenvalue of the equation

$$(-p)^{-1}\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\right)\theta = \lambda_0\theta. \tag{31}$$

Evidently Q is positive-definite provided $\lambda_0 > 1$. From (30) it follows that

$$T = \frac{\mathrm{d}}{\mathrm{d}r} + \tau(r), \qquad T^* = -\frac{\mathrm{d}}{\mathrm{d}r} + \tau(r) \tag{32}$$

where $\tau(r)$ is a short-range function of r which depends on $p(r)$. It is not necessary to find $\tau(r)$, since to evaluate the boundary terms in expressions (12) to (14) we merely need to know the nature of T when r is large.

We now apply the theory of § 2 with

$$f = 0, \qquad \sigma_T = 1 \tag{33}$$

taking trial functions Φ_1 and Φ_2 which satisfy the boundary conditions (20) and (24). The resulting bounds for A are readily seen to be

$$A_-'(\Phi_2) \leqslant A \leqslant A_+'(\Phi_1) \tag{34}$$

where

$$A_+'(\Phi_1) = a_1 + \int_0^\infty \Phi_1\left(p - \frac{\mathrm{d}^2}{\mathrm{d}r^2}\right)\Phi_1 \,\mathrm{d}r \tag{35}$$

and

$$A_-'(\Phi_2) = A_+'(\Phi_2) + (\lambda_0 - 1)^{-1}\int_0^\infty p^{-1}(p\Phi_2 - \Phi_2'')^2 \,\mathrm{d}r \qquad (\lambda_0 > 1). \tag{36}$$

The upper bound (35) is that due to Spruch and Rosenberg (1959), being identical to the expression in (26), while the lower bound (36) appears to be new.

4. Integral equation approach

We next turn to the IE approach specified by equations (3) and (5). It is more convenient to rewrite (3) in the form

$$(p + K)\phi = -rp \tag{37}$$

where K is the symmetric positive-definite integral operator defined by

$$K\psi(r) = \int_0^\infty p(r)\min\{r, r'\}p(r')\psi(r')\,\mathrm{d}r'. \tag{38}$$

Equation (37) can be identified with (6) in various ways, which we consider separately. In all of these ways the operators T and T^* are given by condition (10), so that

$$\sigma_T = 0 \tag{39}$$

and no boundary terms appear in expressions (12) to (14) for I, J and G. Thus T and T^* only occur in the product T^*T, and individual representations of them are not required. All we need is the result that any symmetric positive-definite operator can be decomposed into a product T^*T (Mikhlin 1964). We note that, from equation (39), condition (15) is automatically satisfied.

4.1. *Positive p; $Q = p$*

For positive potentials the straightforward choice is

$$T^*T = K, \qquad Q = p, \qquad f = -rp. \tag{40}$$

Using equations (5) and (11) to (14), (40) leads to

$$B_-(\Phi_1) \leqslant A \leqslant B_+(\Phi_2) \tag{41}$$

where

$$B_+(\Phi_2) = \int_0^\infty \{\Phi_2 K\Phi_2 + p^{-1}(rp + K\Phi_2)^2\}\,\mathrm{d}r \tag{42}$$

and

$$B_-(\Phi_1) = -\int_0^\infty \{2rp\Phi_1 + \Phi_1(p+K)\Phi_1\}\,\mathrm{d}r. \tag{43}$$

The lower bound (43) is due to Schwinger, while the upper bound (42) was derived by Arthurs (1968).

4.2. *Positive p; $Q = (1+\lambda_0)K$*

An alternative way of identifying equation (37) with (6) is to decompose $(p+K)$ into the form $(Q+T^*T)$ by taking.

$$Q = (1+\lambda_0)K, \qquad T^*T = p-\lambda_0 K \tag{44}$$

where λ_0 is the smallest eigenvalue of

$$K^{-1}p\theta = \lambda_0\theta \tag{45}$$

(λ_0 is the same number as that specified by equation (31) in § 3.2). Then again with

$$f = -rp \tag{46}$$

we obtain

$$C_-(\Phi_1) \leqslant A \leqslant C_+(\Phi_2) \tag{47}$$

where the lower bound $C_-(\Phi_1)$ is the same as in equation (43). The alternative upper bound

$$C_+(\Phi_2) = \int_0^\infty \Phi_2(p-\lambda_0 K)\Phi_2\,\mathrm{d}r$$
$$+(1+\lambda_0)^{-1}\int_0^\infty \{pr+(p-\lambda_0 K)\Phi_2\}K^{-1}\{pr+(p-\lambda_0 K)\Phi_2\}\,\mathrm{d}r \tag{48}$$

seems to be new.

4.3. *Negative p; $Q = (1-\lambda_0{}^{-1})(-p)$*

For negative potentials a suitable choice is

$$T^*T = -(p\lambda_0{}^{-1}+K), \qquad Q = (1-\lambda_0{}^{-1})(-p), \qquad f = rp \tag{49}$$

where we now think of λ_0 as the smallest eigenvalue of

$$\lambda_0(-p)^{-1}K\theta = \theta. \tag{50}$$

Thus Q is positive-definite provided again that $\lambda_0 > 1$. Using equations (5) and (11)–(14), we find that (49) leads to

$$B_-'(\Phi_2) \leqslant A \leqslant B_+'(\Phi_1) \tag{51}$$

where

$$B_+'(\Phi_1) = -\int_0^\infty \{2rp\Phi_1 + \Phi_1(p+K)\Phi_1\}\,dr \tag{52}$$

and

$$B_-'(\Phi_2) = \int_0^\infty \Phi_2(p\lambda_0^{-1}+K)\Phi_2\,dr + \frac{\lambda_0}{\lambda_0-1}\int_0^\infty \{rp+(p\lambda_0^{-1}+K)\Phi_2\} \times p^{-1}\{rp+(p\lambda_0^{-1}+K)\Phi_2\}\,dr \qquad (\lambda_0 > 1). \tag{53}$$

The upper bound (52) is due to Schwinger, while the lower bound (53) is contained in a result of Arthurs (1968).

4.4. *Negative p; $Q = (\lambda_0 - 1)K$*

An alternative decomposition to (49) is provided by taking

$$T^*T = -(p+\lambda_0 K), \qquad Q = (\lambda_0-1)K, \qquad f = rp \tag{54}$$

where λ_0 is the number defined in equation (50). Once again Q is positive-definite provided that $\lambda_0 > 1$. Using equations (5) and (11)–(14), we find that (54) leads to

$$C_-'(\Phi_2) \leqslant A \leqslant C_+'(\Phi_1) \tag{55}$$

where the upper bound $C_+'(\Phi_1)$ is given by the Schwinger expression (52), and the lower bound $C_-'(\Phi_2)$ is given by

$$C_-'(\Phi_2) = \int_0^\infty \Phi_2(p+\lambda_0 K)\Phi_2\,dr - (\lambda_0-1)^{-1}\int_0^\infty \{rp+(p+\lambda_0 K)\Phi_2\} \times K^{-1}\{rp+(p+\lambda_0 K)\Phi_2\}\,dr \qquad (\lambda_0 > 1) \tag{56}$$

which appears to be new.

5. Illustrative results

To illustrate the theory we have calculated bounds on scattering lengths for both positive and negative screened Coulomb potentials given by

$$V(r) = \{\exp(-\beta r)\}/r \qquad \text{and} \qquad V(r) = -\{\exp(-\beta r)\}/r \tag{57}$$

β being some positive parameter. The scattered particle was chosen to have mass $m = 1$ A.U. and the following trial functions were used:

$$\text{D.E. approach} = a\{1-\exp(-\alpha r)\} - r \tag{58}$$

$$\text{I.E. approach} = a\{1-\exp(-r)\} - r\{1-\exp(-r)\} \tag{59}$$

where a and α are variational parameters. These functions have the correct behaviour at zero and infinity. The trial function (59), containing a linear variational parameter, is one of the simplest functions that can be employed. It proves to be too inflexible in the D.E. approach as it leads to divergent lower bounds for $\beta \geqslant 2$, but this shortcoming is readily avoided by using the trial function (58). Calculations have been performed for a range of values of β and the results (in atomic units) are shown in tables 1 and 2. For some bounds, C_+, A_-', B_-' and C_-', the eigenvalue λ_0 was

Table 1. Upper and lower bounds on scattering lengths for $V = \{\exp(-\beta r)\}/r$

β	A_-	A_+	B_-	B_+	C_-	C_+
1	1·0443	1·0595	1·0522	1·0587	1·0522	1·1126
2	0·33902	0·34058	0·34044	0·34053	0·34044	0·34919
3	0·16817	0·16855	0·16854	0·16854	0·16854	0·18006
5	0·066920	0·066980	0·066974	0·066974	0·066974	0·079333
10	0·018201	0·018206	0·018204	0·018204	0·018204	0·027764

Table 2. Upper and lower bounds on scattering lengths for $V = -\{\exp(-\beta r)\}/r$

β	A_-'	A_+'	B_-'	B_+'	C_-'	C_+'
2	−1·2359	−1·1030	−1·1121	−1·0967	−1·1709	−1·0967
3	−0·36850	−0·34321	−0·34321	−0·34232	−0·36615	−0·34232
5	−0·10501	−0·10082	−0·10114	−0·10072	−0·12414	−0·10072
10	−0·022704	−0·022260	−0·022260	−0·022255	−0·039693	−0·022255

required. This was calculated by an iteration method (Morse and Feshbach 1963, Anderson and Robinson, to be published) giving

$$\lambda_0 = \beta(0.839\,690\,95). \tag{60}$$

The condition $\lambda_0 > 1$ which must be satisfied (see § 4) in A_-', B_-' and C_-' therefore places a lower limit on possible values of β in these cases.

6. Discussion

Upper and lower bounds on scattering lengths have been obtained by decompositions based on differential and integral equation approaches. Judging by the results in tables 1 and 2 we see that in the positive potential case the B_- of Schwinger in equation (43) and the B_+ bound in equation (42) are better than the other bounds, while in the negative potential case the A_+' bound of Spruch and Rosenberg in equation (35) and the B_-' bound in equation (53) give the best results. In general, because of smoothing effects, we expect bounds involving integral operators to be better than bounds involving differential operators, and so for a given trial function the B bounds should be better than the A and C bounds.

In a subsequent communication it is hoped to extend the analysis to the case of non-zero energy.

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