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Upper and lower bounds on generalized scattering lengths

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

1. Introduction

Upper and lower bounds for the ordinary scattering length A_0 have recently been derived from the theory of complementary variational principles using both the differential and integral equation formulations (Arthurs 1968, Anderson *et al.* 1970). An extension of these results to allow for general values of the orbital angular momentum is of some interest and in this paper we derive upper and lower bounds for generalized scattering lengths A_L.

All the results follow from the general theory for a certain class of linear operator equations. They are illustrated with calculations in the cases $L = 1$ and $L = 2$ for both positive and negative screened Coulomb potentials.

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

$$\left\{-\frac{d^2}{dr^2}+\frac{L(L+1)}{r^2}+p(r)\right\}\phi(r)=0 \qquad 0\leqslant r<\infty \tag{1}$$

subject to the conditions

$$\phi(0)=0 \qquad \phi(r)\sim A_L\frac{(2L-1)!!}{r^L}-\frac{r^{L+1}}{(2L+1)!!} \qquad \text{as } r\to\infty \tag{2}$$

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

$$\phi(r)=-\frac{r^{L+1}}{(2L+1)!!}-\int_0^\infty k(r,r')p(r')\phi(r')\,dr' \tag{3}$$

where

$$k(r,r^1)=\frac{1}{2L+1}\frac{{r_<}^{L+1}}{{r_>}^{L}} \qquad r_<=\min(r,r^1) \qquad r_>=\max(r,r^1) \tag{4}$$

and

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

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

$$A_L=-\frac{1}{(2L+1)!!}\int_0^\infty r^{L+1}p(r)\phi(r)\,dr \qquad L=0,1,2,\ldots. \tag{6}$$

2. General theory

Our results follow from the general theory for a certain class of linear operator equations, which we include here for completeness.

We consider a physical problem which is described by the equation

$$(T^*T+Q)\phi = f \qquad 0 \leqslant r < \infty \tag{7}$$

with

$$\phi = \phi_{\mathrm{B}} \qquad \text{on the boundary of } (0,\ \infty). \tag{8}$$

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

$$\int_0^\infty uT\phi \, \mathrm{d}r = \int_0^\infty (T^*u)\phi \, \mathrm{d}r + \Big[u\sigma_T\phi\Big]_0^\infty \tag{9}$$

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

$$\text{(i) } T = \frac{\mathrm{d}}{\mathrm{d}r} + \frac{L}{r} + \tau(r) \qquad T^* = -\frac{\mathrm{d}}{\mathrm{d}r} + \frac{L}{r} + \tau(r) \qquad \sigma_T = 1 \tag{10}$$

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

$$\text{(ii) } T = \text{integral operator} \qquad T^* = \text{adjoint integral operator} \qquad \sigma_T = 0. \tag{11}$$

Complementary variational principles associated with certain boundary value problems have been developed recently (cf. Arthurs 1970). For problems described by equations (7) and (8) these principles lead to upper and lower bounds

$$G(T\Phi_2) \leqslant I(\phi) \leqslant J(\Phi_1) \tag{12}$$

for the functional

$$I(\phi) = -\tfrac{1}{2}\int_0^\infty f\phi \, \mathrm{d}r + \tfrac{1}{2}[(T\phi)\sigma_T\phi]_0^\infty . \tag{13}$$

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

$$J(\Phi_1) = \tfrac{1}{2}\int_0^\infty \Phi_1(T^*T+Q)\Phi_1 \, \mathrm{d}r - \int_0^\infty f\Phi_1 \, \mathrm{d}r - [(T\Phi_1)\sigma_T(\tfrac{1}{2}\Phi_1 - \phi_{\mathrm{B}})]_0^\infty \tag{14}$$

and

$$G(T\Phi_2) = -\tfrac{1}{2}\int_0^\infty \Phi_2 T^*T\Phi_2 \, \mathrm{d}r - \tfrac{1}{2}\int_0^\infty (f - T^*T\Phi_2)Q^{-1}(f - T^*T\Phi_2) \, \mathrm{d}r - [(T\Phi_2)\sigma_T(\tfrac{1}{2}\Phi_2 - \phi_{\mathrm{B}})]_0^\infty . \tag{15}$$

From these expressions for J and G it can be verified directly that the bounds in equation (12) hold good, provided that the trial function Φ_1 satisfies

$$[T(\Phi_1 - \phi)\sigma_T(\Phi_1 - \phi_{\mathrm{B}})]_0^\infty \leqslant 0. \tag{16}$$

3. Differential equation approach

We now apply the theory of § 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 (7) and (8). It is convenient to treat the cases $p>0$ and $p<0$ separately.

3.1. *The case* $p>0$

We choose

$$T=\frac{\mathrm{d}}{\mathrm{d}r}+\frac{L}{r} \qquad T^*=-\frac{\mathrm{d}}{\mathrm{d}r}+\frac{L}{r} \qquad \sigma_T=1 \tag{17}$$

$$Q=p \qquad f=0 \tag{18}$$

$$\phi_{\mathrm{B}}=0 \text{ at } r=0 \qquad \phi_{\mathrm{B}}\sim A_L\frac{(2L-1)!!}{r^L}-\frac{r^{L+1}}{(2L+1)!!} \quad \text{as } r\to\infty. \tag{19}$$

Then the results of § 2 apply to equations (1) and (2), provided condition (16) is satisfied. The optimum choice for this condition becomes

$$\left[(\Phi_1-\phi_{\mathrm{B}})\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{L}{r}\right)(\Phi_1-\phi)\right]_0^\infty=0. \tag{20}$$

We shall satisfy (20) by taking the trial function Φ_1 such that

$$\Phi_1(0)=0 \qquad \Phi_1\sim a_1\frac{(2L-1)!!}{r^L}-\frac{r^{L+1}}{(2L+1)!!} \quad \text{as } r\to\infty \tag{21}$$

where a_1 is a constant. The basic functionals in (13), (14) and (15) then become

$$I(\phi)=\tfrac{1}{2}\left(\frac{R^{2L+1}}{(2L-1)!!\,(2L+1)!!}-A_L\right)_{R\to\infty} \tag{22}$$

$$J(\Phi_1)=\tfrac{1}{2}\int_0^\infty \Phi_1\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{L(L+1)}{r^2}+p\right)\Phi_1\,\mathrm{d}r + \tfrac{1}{2}\left\{\frac{R^{2L+1}}{(2L-1)!!\,(2L+1)!!}+a_1-2A_L\right\}_{R\to\infty} \tag{23}$$

and

$$G(T\Phi_2)=-\tfrac{1}{2}\int_0^\infty \Phi_2\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{L(L+1)}{r^2}\right)\Phi_2\,\mathrm{d}r -\tfrac{1}{2}\int_0^\infty p^{-1}\left\{\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{L(L+1)}{r^2}\right)\Phi_2\right\}^2\mathrm{d}r - \left[(\tfrac{1}{2}\Phi_2-\phi_{\mathrm{B}})\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{L}{r}\right)\Phi_2\right]_0^\infty. \tag{24}$$

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

$$\Phi_2(0)=0 \qquad \Phi_2\sim a_2\frac{(2L-1)!!}{r^L}-\frac{r^{L+1}}{(2L+1)!!} \quad \text{as } r\to\infty \tag{25}$$

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

$$A_-(\Phi_2) \leqslant A_L \leqslant A_+(\Phi_1) \tag{26}$$

where

$$A_+(\Phi_1) = a_1 + \int_0^\infty \Phi_1 \left(-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + p\right) \Phi_1 \, dr \tag{27}$$

and

$$A_-(\Phi_2) = a_2 - \int_0^\infty \left\{\left(-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2}\right) \Phi_2\right\} p^{-1}$$

$$\times \left\{\left(-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + p\right) \Phi_2\right\} dr. \tag{28}$$

The upper bound (27) is the non-zero L form of the one due to Spruch and Rosenberg (1959), while the lower bound (28) is a generalization of a result of Anderson *et al.* (1970).

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. We retain the identification

$$-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + p = T^*T + Q \tag{29}$$

but this time we take

$$T^*T = -\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + \lambda_0 p \tag{30}$$

$$Q = (\lambda_0 - 1)(-p) \tag{31}$$

where λ_0 is the lowest eigenvalue of the equation

$$(-p)^{-1} \left(-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2}\right) \theta = \lambda_0 \theta. \tag{32}$$

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

$$T = \frac{d}{dr} + \frac{L}{r} + \tau(r) \qquad T^* = -\frac{d}{dr} + \frac{L}{r} + \tau(r) \tag{33}$$

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 (13) to (15) we merely need to know the nature of T when r is large.

We now apply the theory of § 2 with

$$f = 0 \qquad \sigma_T = 1 \tag{34}$$

taking trial functions Φ_1 and Φ_2 which satisfy the boundary conditions (21) and (25). The resulting bounds for A_L are found to be

$$A_-'(\Phi_2) \leqslant A_L \leqslant A_+'(\Phi_1) \tag{35}$$

where

$$A_+'(\Phi_1) = a_1 + \int_0^\infty \Phi_1 \left(-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + p\right) \Phi_1 \, dr \tag{36}$$

and

$$A_-'(\Phi_2) = a_2 + (\lambda_0 - 1)^{-1} \int_0^\infty \left\{\left(-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + \lambda_0 p\right) \Phi_2\right\} p^{-1} \times \left\{\left(-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + p\right) \Phi_2\right\} dr \qquad (\lambda_0 > 1). \tag{37}$$

The upper bound (36) is the non-zero L form of that due to Spruch and Rosenberg (1959), being identical to the expression in (27), while the lower bound (37) is a generalization of a result of Anderson *et al.* (1970).

4. Integral equation approach

We now turn to the integral equation approach specified by equations (3) and (6). It is more convenient to rewrite (3) in the form

$$(K+p)\phi = -\frac{pr^{L+1}}{(2L+1)!!} \tag{38}$$

where K is the symmetric positive integral operator defined by

$$K\psi(r) = \int_0^\infty p(r) k(r, r') \, p(r') \, \psi(r') \, dr' \tag{39}$$

with

$$k(r, r') = \frac{1}{2L+1} \frac{r_<^{L+1}}{r_>^L} \qquad r_< = \min(r, r') \qquad r_> = \max(r, r'). \tag{40}$$

Equation (38) can be identified with (7) in various ways, which we consider separately. In each of these ways the operators T and T^* are given by condition (11), so that

$$\sigma_T = 0 \tag{41}$$

and no boundary terms appear in expressions (13) to (15) 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 operator can be decomposed into a product T^*T (Mikhlin 1964). Note that, from equation (41), condition (16) is automatically satisfied.

4.1. *Positive p*

For positive potentials we choose

$$T^*T = K \qquad Q = p \qquad f = -\frac{pr^{L+1}}{(2L+1)!!}. \tag{42}$$

Using equations (6) and (12) to (15) we find that (42) leads to

$$B_-(\Phi_1) \leqslant A_L \leqslant B_+(\Phi_2) \tag{43}$$

where

$$B_+(\Phi_2) = \int_0^\infty \left\{\Phi_2 K \Phi_2 + p^{-1} \left(\frac{pr^{L+1}}{(2L+1)!!} + K\Phi_2\right)^2\right\} dr \tag{44}$$

and

$$B_-(\Phi_1) = -\int_0^\infty \left(\frac{2pr^{L+1}}{(2L+1)!!}\Phi_1 + \Phi_1(K+p)\Phi_1\right) dr. \tag{45}$$

The lower bound (45) is the non-zero L form of the Schwinger bound (cf. Moiseiwitsch 1966), while the upper bound (44) is a generalization of a result derived by Arthurs (1968).

4.2. *Negative p*

For negative potentials a suitable choice is

$$T^*T = -(p\lambda_0^{-1}+K) \qquad Q = (1-\lambda_0^{-1})(-p) \qquad f = \frac{pr^{L+1}}{(2L+1)!!} \tag{46}$$

where we now think of λ_0 as the smallest eigenvalue of

$$\lambda_0(-p)^{-1}K\theta = \theta. \tag{47}$$

Thus Q is positive provided again that $\lambda_0 > 1$. Using equations (6) and (12) to (15) we find that (46) leads to

$$B_-'(\Phi_2) \leqslant A_L \leqslant B_+'(\Phi_1) \tag{48}$$

where

$$B_+'(\Phi_1) = -\int_0^\infty \left(\frac{2pr^{L+1}}{(2L+1)!!}\Phi_1 + \Phi_1(K+p)\Phi_1\right) dr \tag{49}$$

and

$$B_-'(\Phi_2) = \int_0^\infty \Phi_2(p\lambda_0^{-1}+K)\Phi_2\, dr + \frac{\lambda_0}{\lambda_0 - 1}\int_0^\infty p^{-1} \times \left(\frac{pr^{L+1}}{(2L+1)!!} + (p\lambda_0^{-1}+K)\Phi_2\right)^2 dr \qquad (\lambda_0 > 1). \tag{50}$$

The upper bound (49) is the non-zero L form of the Schwinger bound, while the lower bound (50) is a generalization of a result of Arthurs (1968).

5. Illustrative results

To illustrate the theory we have calculated bounds on generalized scattering lengths A_L for $L = 1$ and $L = 2$ from the differential equation approach for both positive and negative screened Coulomb potentials given by

$$V(r) = \{\exp(-\beta r)\}/r \qquad \text{and} \qquad V(r) = -\{\exp(-\beta r)\}/r \tag{51}$$

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

$$\Phi = a(2L-1)!!\, r^{-L}\{1 - \exp(-\alpha r)\}^{2L+1} - \frac{r^{L+1}}{(2L+1)!!} \tag{52}$$

where a and α are variational parameters. This function has the correct behaviour at zero and infinity. Calculations have been performed for $L = 1$ and $L = 2$ and a range of values of β, and the results (in atomic units) are shown in tables 1 and 2. The $L = 0$ bounds of Anderson *et al.* (1970) are included for comparison purposes. For the bound A_-' the eigenvalues λ_0 corresponding to $L = 1$ and $L = 2$ were

Table 1. Upper and lower bounds on A_0, A_1 and A_2 for $V = \{\exp(-\beta r)\}/r$

β	$A_-(L=0)$	$A_+(L=0)$	$A_-(L=1)$	$A_+(L=1)$	$A_-(L=2)$	$A_+(L=2)$
1	1·0443	1·0595	1·1809	1·2373	0·90375	1·0539
2	0·33902	0·34058	0·77133(−1)	0·80118(−1)	0·14313(−1)	0·16565(−1)
3	0·16817	0·16855	0·15474(−1)	0·16027(−1)	0·12623(−2)	0·14572(−2)
5	0·66920(−1)	0·66980(−1)	0·20310(−2)	0·20989(−2)	0·59110(−4)	0·68098(−4)
10	0·18201(−1)	0·18206(−1)	0·12817(−3)	0·13224(−3)	0·92614(−6)	0·10653(−5)

Table 2. Upper and lower bounds on A_0, A_1 and A_2 for $V = -\{\exp(-\beta r)\}/r$

β	$A_-'(L=0)$	$A_+'(L=0)$	$A_-'(L=1)$	$A_+'(L=1)$	$A_-'(L=2)$	$A_+'(L=2)$
1	—	—	−1·4703	−1·4663	−1·0889	−1·0806
2	−1·2359	−1·1030	−0·87237(−1)	−0·87109(−1)	−0·16836(−1)	−0·16773(−1)
3	−0·36850	−0·34321	−0·16961(−1)	−0·16944(−1)	−0·14731(−2)	−0·14694(−2)
5	−0·10501	−0·10082	−0·21714(−2)	−0·21700(−2)	−0·68541(−4)	−0·68438(−4)
10	−0·22704(−1)	−0·22260(−1)	−0·13450(−3)	−0·13446(−3)	−0·10688(−5)	−0·10680(−5)

Here $N(-m)$ means $N \times 10^{-m}$.

required. These were calculated by an iteration method (cf. Robinson *et al.*, 1970) and found to be

$$\lambda_0(L = 1) = 4{\cdot}5396\,\beta \qquad \lambda_0(L = 2) = 10{\cdot}941\,\beta. \tag{53}$$

The condition $\lambda_0 > 1$ which must be satisfied (see §§ 3 and 4) in A_-' and B_-' therefore places a lower limit on possible values of β in these cases.

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