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The least norm method: upper and lower bounds for scattering phase shifts

E J Kanellopoulos and Th V Kanellopoulos

Institut für Theoretische Physik der Universität Tübingen, Tübingen, Germany

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Abstract. A variational method is presented which is based on the minimization of the norm of the function $H-E|\psi\rangle$ and therefore can be considered as a generalization of the recently developed methods by Harris, Ladányi and Schmid. It seems more laborious than the above methods but it can be used with confidence when there does not exist, *a priori*, any information about the expected results. It is free of singularities, the results are obtained in terms of absolutely converging series and it provides criteria for choosing the components of the trial function.

On the other hand it leads in a straightforward way to a simple formalism for upper and lower bounds of the phase shifts. This formalism needs a reasonable amount of calculation; it is easily applicable to one- or many-channel scattering as well as to the cases where exchange effects are taken into account

1. Introduction

A method for attacking in an approximate way a complicated problem will be called 'effective' if at the same time it provides a kind of criterion by which one can either find out which of two different results obtained by this method is closer to the correct one, or estimate the corresponding probable error. Such an 'effective' method, for example, is the Ritz–Schrödinger (RS) variational method for the calculation of energy levels. This is due to the fact that this method provides an extremum principle.

The RS variational method has been extended to the scattering problems by Hulthén (1944, 1948, 1952), Kohn (1948), Feshbach and Rubinow (1952) and others. These methods however, at least for calculations of phase shifts, are not 'effective'. Extrema principles do not exist and the results obtained by them do not show generally any regular convergence. Moreover the presence of spurious singularities (Schwartz 1961) increases the calculation labour for localizing or eliminating them, while no rule exists for choosing the components of the trial function.

For a period interest was focused towards modifying the above methods in order to avoid the spurious singularities (Harris 1967, Harris and Michels 1967, Nesbet 1968) though without full success. On the other hand the recently developed methods by Harris and Michels (1969), Ladányi and Szondy (1971) and Schmid and Schwager (1972), although avoiding spurious singularities, fail to improve generally the behaviour of the obtainable results or to provide an estimation of the probable error.

Only Kato's (1951) method is an 'effective' one, as it provides upper and lower bounds for the phase shifts. It is applicable to the case of elastic scattering by a central potential. Spruch and Rosenberg (1960) have applied Kato's method to the case of

zero energy e^+H scattering. Unfortunately, it seems that it is not possible to apply this method to the general case of many-channel scattering or to the case when exchange effects are taken into account.

The least norm method (LNM) presented here is free of singularities, derives the results in terms of absolutely convergent series, gives criteria for choosing suitable components of the trial function, provides a measure of the mean deviation of the trial function from the exact solution and, finally, leads in a very simple way to upper and lower bounds for phase shifts. The method is applicable to the case of many-channel scattering and to the case with exchange effects.

The text of this paper falls into two parts. The first part consists of §§ 2 and 3. In § 2 the general trend of the LNM is exposed. For the sake of clarity we consider the case of one-channel scattering by a local central potential—the extension to more complicated cases is straightforward. Suitable ways for application of the method are given in § 3. In all cases explicit expressions for the phase shifts are given in terms of absolutely converging series.

Most important, however, is the second part, § 4, in which one arrives by a simple way at upper and lower bounds for the phase shifts, for one- as well as for many-channel scattering. A numerical application to e^-H^1 scattering in a static approximation is given at the end of § 4 to illustrate the use of the bounds in obtaining quite accurate results, in spite of the fact that the gap between upper and lower bounds could be relatively large. The procedure is as follows. One uses only the linear parameters as variational ones, while the nonlinear ones are left as free parameters. Considering several sets of values for these free parameters one obtains several pairs of bounds. The overlapping of the gaps between the bounds narrows the range in which the phase shift must lie and so one can reach high accuracy.

1.1. The basic concept

The development of the method is based on the following proposition. 'If

$$\int_{\underline{Q}} f^* f \, d\tau = 0 \tag{1}$$

the function f is zero almost everywhere within the region of integration.'

Therefore if one is looking for a solution of any equation of the form

$$\sigma\psi = 0 \tag{2}$$

with given boundary conditions, it is sufficient to state that

$$N^2 = \int_{\underline{Q}} w(r)(\sigma\psi)^\dagger(\sigma\psi) \, d\tau = 0. \tag{3}$$

The integration extends over a region $\underline{Q} \geqslant D$, where D is the region of definition of the solution of equation (2). In the integration (3) care is taken to incorporate the boundary conditions in the function ψ, while $w(r)$ is any function which is positive throughout the region of integration, except perhaps at the origin where it may be zero.

For an approximate solution of (2) the corresponding requirement is that the left-hand side of (3) is a minimum. Therefore in an approximative procedure the problem becomes a variational one and the value of N^2 can be defined as the norm of the function $\sigma\psi$. It gives a measure of the mean deviation from the exact solution. The simplest way

is to use a direct method, ie to expand ψ in terms of a complete set of independent functions in the region of definition of the solutions, taking care to incorporate the boundary conditions. Then the coefficients of the expansion are the variational parameters.

2. The method

2.1. Notation

For simplicity of the formalism we adopt the following notation:

$$\hat{H} = E - H \tag{4}$$

$$\hat{f} = (E-H)f \tag{5}$$

$$(f, g) = \langle f\hat{H}^{+}|w|\hat{H}g\rangle = \langle \hat{f}|w|\hat{g}\rangle = \int w\hat{f}^{*}\hat{g}\,\mathrm{d}\tau. \tag{6}$$

Especially in the case we consider here,

$$\hat{H} = \frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{l(l+1)}{r^2} + v(r) \tag{4a}$$

where the following conditions on $v(r)$ are imposed:

$$\int_0^a r|v(r)|\,\mathrm{d}r < \infty, \qquad \int_a^\infty |v(r)|\,\mathrm{d}r < \infty$$

for any $0 < a < \infty$.

2.2. Form of the trial function: remarks

If we use standing waves and S_l, C_l are the regular and irregular asymptotic solutions of

$$\hat{H}\omega = 0 \tag{7}$$

where H is (4), we put $S = S_l$ and $C = C_l g$. The function g is used to eliminate the singularity of C_l at the origin such that

$$g^{(r)}_{r\to 0} \sim r^{2l+1}, \qquad g^{(r)}_{r\to\infty} \to 1. \tag{8}$$

Then we can write the solution of (7), ω, as

$$\omega = S + xC + \Phi. \tag{9}$$

The function Φ, in as much as $v(r)$ and $\mathrm{d}g(r)/\mathrm{d}r$ fall off at infinity faster than $r^{-3/2}$ (see appendix), is a normalizable real function which behaves at the origin as r^{l+1}. Then x is the tangent of the phase shift η_l. With these requirements in the formation of ω we incorporate in it the proper boundary conditions. Now given any 'complete' set of linearly independent functions $\{u_i\}$, Φ can be expanded as

$$\Phi = \sum_{i=1}^{\infty} a_i u_i. \tag{10}$$

In an approximation one truncates the expansion (10), considering the first n terms of it. The set is 'complete' in the sense that all of its components behave at the origin

as r^m with $m \geqslant l+1$. On this point it is interesting to make the following simple but useful remarks:

(i) Given a complete set of independent functions $\{e_j\}$ $(j = 0, 1, 2, \ldots)$, which span a Hilbert space $\mathscr{H}_0$, one can rearrange it to form the equivalent set $\{u_i\}$ such that

$$u_n = r^n v_n(r) \qquad (n = 0, 1, 2, \ldots)$$

where $0 < |v_n(0)| < \infty$. Any subset $\{u_k\}$ with $k \geqslant m$ spans a subspace $\mathscr{H}_m$. It is obvious that

$$\mathscr{H}_0 \supset \mathscr{H}_1 \supset \mathscr{H}_2 \ldots,$$

and that any subspace $\mathscr{H}_n$ has exactly one dimension more than the next one $\mathscr{H}_{n+1}$.

If we expand the function Φ of (10) in terms of the complete set $\{u_i\}$ $(i = 0, 1, 2, \ldots)$ we shall have

$$\Phi = \sum_{j=0}^{\infty} b_j u_j = \sum_{j=0}^{\infty} b_j r^j v_j.$$

Requiring now that the exact Φ behaves at the origin as r^{l+1} we see at once that

$$b_0 = b_1 = b_2 = \ldots = b_l = 0.$$

Therefore taking u_i in (10) behaving at $r = 0$ at least as r^{l+1} we avoid using components which disappear at the limit.

(ii) While the chosen set $\{u_i\}$ in (10) is a complete set for the subspace $\mathscr{H}_{l+1}$, when we apply the operator $\hat{H}$, because of its kinetic energy part†, we have $\{\hat{u}_i\} \subset \mathscr{H}_l$, and therefore the set $\{\hat{u}_i\}$ is not complete in this subspace. It is missing exactly one dimension. There is one-to-one correspondence between the two sets $\{u_i\} \subset \mathscr{H}_{l+1}$ and $\{\hat{u}_j\} \subset \mathscr{H}_l$. The functions $\hat{S}$ and $\hat{C}$ are normalizable and belong to the subspace $\mathscr{H}_l$ but not to the part of it spanned by the set $\{\hat{u}_i\}$, because then S and C ought to belong to the subspace $\mathscr{H}_{l+1}$, ie should be normalizable. So one can put

$$\hat{S} = \hat{S}_\perp + \hat{S}_\parallel, \qquad \hat{C} = \hat{C}_\perp + \hat{C}_\parallel \tag{11}$$

where

$$\hat{S}_\parallel \text{ and } \hat{C}_\parallel \subset \{\hat{u}_i\}, \tag{12}$$

while

$$\hat{S}_\perp \| \hat{C}_\perp \perp \{\hat{u}_i\}. \tag{13}$$

It is interesting to note that $\hat{C}_\perp$ is not affected by the cut-off function which is introduced in C in order to make it behave as r^{l+1} at the origin.

From the relation

$$\hat{H}\omega = \hat{S} + x\hat{C} + \hat{\Phi}$$

we have

$$(\hat{S}_\perp + x\hat{C}_\perp) + (\hat{S}_\parallel + x\hat{C}_\parallel + \hat{\Phi}) = 0; \tag{14}$$

therefore,

$$x = -\hat{S}_\perp / \hat{C}_\perp \tag{15}$$

and

$$\hat{S}_\parallel + x\hat{C}_\parallel + \hat{\Phi} = 0. \tag{16}$$

† We suppose that $v(r)$ has at most a simple pole at the origin.

In the present method one is working with equation (16) but the final result, at the limit, is the relation (15) in the form

$$x = -\frac{\langle \hat{C}_\perp | \hat{S}_\perp \rangle}{\langle \hat{C}_\perp | \hat{C}_\perp \rangle} = -\frac{\langle \hat{S}_\perp | \hat{S}_\perp \rangle}{\langle \hat{S}_\perp | \hat{C}_\perp \rangle} = -\frac{\langle \hat{C} | \hat{S}_\perp \rangle}{\langle \hat{C} | \hat{C}_\perp \rangle}. \tag{17}$$

The resonances are the special cases for which

$$\hat{C}_\perp \simeq 0. \tag{18}$$

Working with equation (16) is equivalent to approximating the exact solution, while if it were possible to find a function z such that

$$z \perp \{\hat{u}_i\},$$

then one could obtain from (9) directly the phase

$$x = -\langle z | \hat{S} \rangle / \langle z | \hat{C} \rangle.$$

2.3. The method

Using (9) and (10) we have in the nth approximation

$$N_n^2 = (\omega_n, \omega_n) = (S, S) + 2(S, C)x_n + (C, C)x_n^2 + 2\sum_{j=1}^{n} a_j(S, u_j) + 2x_n \sum_{j=1}^{n} a_j(C, u_j)$$

$$+ \sum_{i,j}^{n} a_i a_j (u_i, u_j). \tag{19}$$

This expression, which at the limit $n \to \infty$ is zero, is simply the square of the norm of the function $\hat{\omega}_n = \hat{H}\omega_n$.

The minimum of this norm is obtained when x_n and a_j's fulfil the conditions:

$$\frac{\partial N_n^2}{\partial x_n} = 0, \qquad \frac{\partial N_n^2}{\partial a_j} = 0 \qquad (j = 1, 2, \ldots, n)$$

or explicitly

$$(S, C) + x_n(C, C) + \sum_{i=1}^{n} a_i(C, u_i) = (C, \omega_n) = 0 \tag{19a}$$

$$(S, u_j) + x_n(C, u_j) + \sum_{i=0}^{n} a_i(u_j, u_i) = (u_j, \omega_n) = 0 \qquad j = 1, 2, \ldots, n. \tag{19b}$$

Then as $N_n^2 = (\omega_n, \omega_n)$, taking into account (19) we have:

$$N_n^2 = (\omega_n, \omega_n) = (S, \omega_n). \tag{20}$$

Using the notation

$$(i, j) = (u_i, u_j), \qquad D_n^{fg} = \begin{vmatrix} (f, g) & (f, 1) \ldots (f, n) \\ (1, g) & (1, 1) \ldots (1, n) \\ \vdots & \vdots \quad \vdots \\ (n, g) & (n, 1) \ldots (n, n) \end{vmatrix} \qquad \text{and} \qquad D_n = \det(i, j)$$

we find from (19):

$$x_n = -D_n^{SC}/D_n^{CC} \tag{21}$$

and

$$D_n N_n^2 = D_n^{CC} x_n^2 + 2D_n^{SC} x_n + D_n^{SS}. \tag{22}$$

In (22) only the a_{ij}'s are eliminated among (19). Its minimum is given by

$$D_n N_{n,\min}^2 = D_n^{SS} - (D_n^{SC})^2/D_n^{CC}. \tag{23}$$

As $\{u_i\}$ (or equivalently $\{\hat{u}_i\}$) are linearly independent, and provided that $\hat{S}_\perp \neq 0$ and $\hat{C}_\perp \neq 0$, the determinants D_n, D_n^{CC} and D_n^{SS} are definite positive.

The expressions (21)–(23) are greatly simplified if from the set $\{u_i\}$ we form the equivalent one $\{\chi_j\}$ by putting

$$\chi_1 = u_1/\sqrt{(1,1)}, \qquad \chi_n = \begin{vmatrix} u_1 & u_2 & \dots u_n \\ (1,1) & (1,2) & \dots (1,n) \\ \vdots & \vdots & \vdots \\ (n-1,1) & (n-1,2) & \dots (n-1,n) \end{vmatrix} (D_n D_{n-1})^{-1/2}. \tag{24}$$

Then we have

$$(\chi_m, \chi_n) = \delta_{mn}$$

and

$$\begin{aligned} D_n^{CC} &= (C,C) - \sum_{i=1}^{n} (C,\chi_i)^2 \\ D_n^{SC} &= (S,C) - \sum_{i=1}^{n} (S,\chi_i)(C,\chi_i), \qquad D_n = 1 \\ D_n^{SS} &= (S,S) - \sum_{i=1}^{n} (S,\chi_i)^2 \end{aligned} \tag{25}$$

and (21) becomes

$$x_n = -\left((S,C) - \sum_{i=1}^{n} (S,\chi_i)(C,\chi_i)\right)\left((C,C) - \sum_{i=1}^{n} (C,\chi_i)^2\right)^{-1}. \tag{21a}$$

It is important to notice that

$$\begin{aligned} D_{n+1}^{CC} &= D_n^{CC} - (C,\chi_{n+1})^2 \\ D_{n+1}^{SC} &= D_n^{SC} - (S,\chi_{n+1})(C,\chi_{n+1}) \\ D_{n+1}^{SS} &= D_n^{SS} - (S,\chi_{n+1})^2. \end{aligned}$$

Therefore at the limit $n \to \infty$ we can write

$$x = -\left((S,C) - \sum_{i=1}^{\infty} (S,\chi_i)(C,\chi_i)\right)\left((C,C) - \sum_{i=1}^{\infty} (C,\chi_i)^2\right)^{-1}. \tag{26}$$

Also we have

$$N^2_{\infty,\min} = (S,S) - \sum_{i=1}^{\infty} (S,\chi_i)^2 - \left((S,C) - \sum_{i=1}^{\infty} (S,\chi_i)(C,\chi_i)\right)^2 \left((C,C) - \sum_{i=1}^{\infty} (C,\chi_i)^2\right)^{-1} = 0,$$

ie

$$(S,S) - \sum_{i=1}^{\infty} (S,\chi_i)^2 + x\left((S,C) - \sum_{i=1}^{\infty} (S,\chi_i)(C,\chi_i)\right) = 0, \tag{27}$$

from which again:

$$x = -\left((S,S) - \sum_{i=1}^{\infty} (S,\chi_i)^2\right)\left((S,C) - \sum_{i=1}^{\infty} (S,\chi_i)(C,\chi_i)\right)^{-1}. \tag{28}$$

The series in (26)–(28) are absolutely convergent.

In cases near a resonance we see from (26) and (28) that both terms of (26) tend to zero, so one has to use (28). That both terms of (26) tend to zero is expected from remark (ii) in § 2.2, as then $\hat{C}_\perp = 0$. Now as

$$\hat{C}_\perp = \hat{C} - \sum_{i=1}^{\infty} (C,\chi_i)\hat{\chi}_i$$

and

$$\hat{S}_\perp = \hat{S} - \sum_{i=1}^{\infty} (S,\chi_i)\hat{\chi}_i$$

one can identify formulae (26) and (28) with (17).

Finally the exact wavefunction ω takes the form

$$\omega = \left(S - \sum_{i=1}^{\infty} (S,\chi_i)\chi_i\right) + x\left(C - \sum_{i=1}^{\infty} (C,\chi_i)\chi_i\right). \tag{29}$$

2.4. Choice of the components of the trial function

For the applications one has to choose the functions u_i or χ_i in such a way that the series appearing in (26) or (28) converge quickly.

Equation (22), using (25), becomes

$$N_n^2 = \left((S,S) - \sum_{i=1}^{n} (S,\chi_i)^2\right) + 2x\left((S,C) - \sum_{i=1}^{n} (S,\chi_i)(C,\chi_i)\right) + x^2\left((C,C) - \sum_{i=1}^{n} (C,\chi_i)^2\right).$$

This is a parabola in the (x, N^2) plane. As

$$N_n^2 - N_{n+1}^2 = [(s,\chi_{n+1}) + x(C,\chi_{n+1})]^2 \tag{30}$$

the two consecutive parabolas are tangential in their common point,

$$x = -(S,\chi_{n+1})/(C,\chi_{n+1}). \tag{31}$$

Therefore if one demands that (30) is maximum for some value of x different from that of (31), then N_{n+1}^2 decreases faster and one approaches the exact solution more closely. Putting $x = 0$ in (30) we have

$$(S,\chi_{n+1})^2 = \text{maximum}. \tag{32}$$

If on the other hand we have in (30) $x = x_n$, ie the value of x for which N_n^2 is a minimum, we have the condition

$$[(S, \chi_{n+1}) + x_n(C, \chi_{n+1})]^2 = \text{maximum.} \tag{32a}$$

Either of conditions (32), (32*a*) leads to faster convergence of the series in (26) and (28). Note that in every χ_i only one new function from the set $\{u_i\}$ is included, so in each step of the approximation we can fulfil conditions (32), (32*a*) by parametric adjustment in one function of $\{u_i\}$. In order to avoid complications from the point of view that by varying parameters (linear or not) in $\{u_i\}$ one could arrive at a set of non-independent functions, it is advisable for the functions u_i to be taken in the form

$$u_n = r^{n+l} v_n \qquad (n = 1, 2, \ldots)$$

with $0 < |v_n(0)| < \infty$.

3. Modifications of the method

3.1. One-component procedure

From the complete set $\{u_i\}$ of independent functions one constructs the equivalent one $\{v_j\}$ as follows.

Assuming that $(u_1, C) \neq 0$ we put

$$v_1 = u_1, \qquad v_n = (1, C)u_n - (n, C)u_1.$$

The set $\{v_j\}$ $(j = 1, 2, \ldots)$ is equivalent to the set $\{u_i\}$ and moreover

$$(v_j, C) = 0 \qquad \text{for } j \geqslant 2.$$

Next we construct the equivalent set $\{\chi_j\}$ by taking

$$\chi_2 = v_2, \qquad \chi_n = \begin{vmatrix} v_2 & v_3 & \ldots v_n \\ (v_2, v_2) & (v_2, v_3) & \ldots (v_2, v_n) \\ \vdots & \vdots & \vdots \\ (v_{n-1}, v_2) & (v_{n-1}, v_3) & \ldots (v_{n-1}, v_n) \end{vmatrix} \qquad n \geqslant 3$$

and

$$\chi_1 = u_1 - \sum_{j=2}^{\infty} \frac{(u_1, \chi_j)}{(\chi_j, \chi_j)} \chi_j.$$

It is easy to see that

$$(\chi_m, \chi_n) = 0 \qquad \text{for } m \neq n.$$

Then we can express the exact solution as

$$\omega = S + xC + \sum_{j=1}^{\infty} a_j \chi_j.$$

Using now the conditions

$$(C, \omega) = 0 \qquad \text{and} \qquad (\chi_1, \omega) = 0$$

one finds

$$(C, S)+x(C, C)+a_1(C, \chi_1) = 0$$

$$(\chi_1, S)+x(\chi_1, C)+a_1(\chi_1, \chi_1) = 0,$$

from which

$$x = -[(C, S)(\chi_1, \chi_1)-(C, \chi_1)(S, \chi_1)]/[(C, C)(\chi_1, \chi_1)-(C, \chi_1)^2] \tag{33}$$

with

$$(C, \chi_1) = (C, u_1); \qquad (\chi_1, \chi_1) = (u_1, u_1)-\sum_{j=2}^{\infty}(u_1\chi_j)^2/(\chi_j\chi_j);$$

$$(\chi_1, S) = (u_1, S)-\sum_{j=2}^{\infty}(u_1\chi_j)(\chi_j, S)/(\chi_j, \chi_j). \tag{34}$$

In this procedure the most convenient way ot choosing the components of the trial function is deduced from the following. If we construct the function Φ_n by taking χ_j only with $j \geqslant 2$ we find for x always that, independently of the number of the components of Φ_n,

$$x_n = -(S, C)/(C, C),$$

while the minimum norm becomes

$$N^2_{n,\min} = (S, S)-(S, C)^2/(C, C)-\sum_{i=2}^{n}(S, \chi_i)^2/(\chi_i, \chi_i). \tag{35}$$

So we can write

$$N^2_{n+1,\min} = N^2_{n,\min}-(S, \chi_{n+1})^2/(\chi_{n+1}, \chi_{n+1}),$$

ie in every step of the approximation the minimum of the norm decreases by $(S, \chi_n)^2/(\chi_n, \chi_n)$. Therefore, as $\Sigma_{j=2}^{\infty}(S, \chi_j)^2/(\chi_j, \chi_j) \leqslant (S, S)-(S, C)^2/(C, C)$, in order to have a fast convergence it is enough to require every $(S, \chi_j)^2/(\chi_j, \chi_j)$, $(j \geqslant 2)$, to be maximum. In such a way we quickly arrive at the possible minimum norm by using a number of terms χ_j with $j \geqslant 2$. Then we can turn our attention to the series $\Sigma_{j=2}^{\infty}(u_1, \chi_j)^2/(\chi_j, \chi_j)$, and selecting some more χ_j's, including now χ_1, in such a way that for each of them $(u_1, \chi_j)^2/(\chi_j, \chi_j)$ is again maximum, we complete also the 'saturation' of this series. Then the result obtained from (33) is quite accurate.

3.2. Two-component procedure

Again from a given complete set $\{u_i\}$ of independent functions, supposing that

$$\begin{vmatrix}(1, S) & (2, S)\\ (1, C) & (2, C)\end{vmatrix} \neq 0,$$

we construct the equivalent set

$$v_1 = u_1 \qquad v_2 = u_2 \qquad v_n = \begin{vmatrix} u_1 & u_2 & u_n\\ (1, S) & (2, S) & (n, S)\\ (1, C) & (2, C) & (n, C)\end{vmatrix} \qquad n \geqslant 3,$$

and further the set $\{\chi_j\}$ as:

$$\chi_1 = u_1 - \sum_{j=3}^{\infty} (u_1\chi_j)/(\chi_j\chi_j)\chi_j, \qquad \chi_2 = u_2 - \sum_{j=3}^{\infty} (u_2\chi_j)/(\chi_j\chi_j)\chi_j, \qquad \chi_3 = v_3,$$

$$\chi_n = \begin{vmatrix} v_3 & v_4 & \dots v_n \\ (v_3, v_3) & (v_3, v_4) & \dots (v_3, v_n) \\ \vdots & \vdots & \vdots \\ (v_{n-1}, v_3) & (v_{n-1}, v_4) & \dots (v_{n-1}, v_n) \end{vmatrix} \qquad n \geqslant 3. \tag{36}$$

One then finds that the function Φ in the exact solution has only the components χ_1 and χ_2. Because if we take

$$(\chi_n, \omega) = 0$$

we have

$$(\chi_n, S) + x(\chi_n, C) + a_n(\chi_n, \chi_n) = 0$$

as $(\chi_n, \chi_m) = 0$ for $n \neq m$. Now for $n \geqslant 3$, $(\chi_n, S) = (\chi_n, C) = 0$ and therefore $a_n = 0$, $n \geqslant 3$. So the exact solution is of the form

$$\omega = S + xC + a_1\chi_1 + a_2\chi_2 \tag{37}$$

where the only unknowns are the constants x, a_1 and a_2. As (37) represents the exact solution we shall have

$$\begin{aligned} &(S, S) + x(S, C) + a_1(S, 1) + a_2(S, 2) = 0 \\ &(S, S) + x(C, C) + a_1(C, 1) + a_2(C, 2) = 0 \\ &(1, S) + x(1, C) + a_1(1, 1) + a_2(1, 2) = 0 \\ &(2, S) + x(2, C) + a_1(2, 1) + a_2(2, 2) = 0, \end{aligned} \tag{38}$$

where

$$(S, 1) = (S, u_1), \qquad (S, 2) = (S, u_2), \qquad (C, 1) = (C, u_1), \qquad (C, 2) = (C, u_2)$$

$$(1, 1) = (u_1, u_1) - \sum_{j=3}^{\infty} (u_1, \chi_j)^2/(\chi_j, \chi_j), \qquad (2, 2) = (u_2, u_2) - \sum_{j=3}^{\infty} (u_2, \chi_j)^2/(\chi_j, \chi_j)$$

$$(1, 2) = (u_1, u_2) - \sum_{j=3}^{\infty} (u_1, \chi_j)(u_2, \chi_j)/(\chi_j, \chi_j). \tag{39}$$

These series are also absolutely convergent. By choosing u_1 and u_2 such that $(S, u_1)^2/(u_1, u_1)$ and $(S, u_2)^2/(u_2, u_2)$, or $(C, u_1)^2/(u_1, u_1)$ and $(C, u_2)^2/(u_2, u_2)$, become maxima, we have that their components in the subspace of $\{\chi_j\}, j \geqslant 3$, become as small as possible,and therefore the series (39) converge faster. Then the truncation of these series will introduce small errors in the results.

From system (38) we obtain four values for x which coincide at the limit. In an approximation the largest difference between two of them can be considered as a measure of the error introduced by the truncation of the series.

4. Upper and lower bounds for phase shifts

In this section a simple but quite general method is given by which one derives upper and lower bounds for the phase shifts. In § 4.1 the method is explained for the case of one-channel scattering and in § 4.2 it is extended to many-channel scattering. Some numerical results are given for $e^- H^1$ scattering in the static approximation in § 4.3. The method is applicable also when exchange effects are taken into account and calculations are in progress for low-energy elastic and inelastic scattering of $e^{\pm}$ by a H^1 atom.

4.1. One-channel case

If $\omega = S + xC + af$ is any trial function and we minimize its norm $N^2 = (\omega, \omega)$, we find from (19) and (20):

$$\begin{aligned} &(S,S)+x(S,C)+a(S,f) = N^2 \\ &(C,S)+x(C,C)+a(C,f) = 0 \\ &(f,S)+x(f,C)+a(f,f) = 0. \end{aligned} \tag{40}$$

If instead we consider the system

$$(S,S)+x(S,C)+a(S,f) = 0 \tag{41a}$$

$$(C,S)+x(C,C)+a(C,f) = 0 \tag{41b}$$

$$(f,S)+x(f,C)+a(f,f) = 0, \tag{41c}$$

this system is compatible if and only if

$$D = \begin{vmatrix} (S,S) & (S,C) & (S,f) \\ (S,C) & (C,C) & (C,f) \\ (S,f) & (C,f) & (f,f) \end{vmatrix}. \tag{42}$$

is zero.

From (40) we find that

$$D = N^2 \begin{vmatrix} (C,C) & (C,f) \\ (C,f) & (f,f) \end{vmatrix}. \tag{43}$$

The determinant

$$\begin{vmatrix} (C,C) & (C,f) \\ (C,f) & (f,f) \end{vmatrix}$$

in any stage of approximation is definite positive. For energies near resonances $\hat{C}_\perp \simeq 0$ and the determinant may become very small†. Excluding this case, we have that the system (41) is compatible only when ω is the exact solution. If however

$$(S,S) \gg N^2 = \frac{D}{\begin{vmatrix} (C,C) & (C,f) \\ (C,f) & (f,f) \end{vmatrix}}$$

the system (41) could give approximative values of x.

† In that case we consider as a trial function $\omega = Sy + C + af$ and one can proceed in a similar way.

From (41) one obtains three values for x. We call a 'proper' pair of values those obtained from (41a, 41c) and (41b, 41c). We put

$$x_1 = -A/B, \qquad x_2 = -B/C \tag{44}$$

where

$$A = \begin{vmatrix} (S,S) & (S,f) \\ (S,f) & (f,f) \end{vmatrix}, \qquad B = \begin{vmatrix} (S,C) & (S,f) \\ (C,f) & (f,f) \end{vmatrix}, \qquad C = \begin{vmatrix} (C,C) & (C,f) \\ (C,f) & (f,f) \end{vmatrix}. \tag{45}$$

For any f we have

$$x_1/x_2 = AC/B^2. \tag{46}$$

As

$$AC - B^2 = (f,f)\,.\,D \geqslant 0 \tag{47}$$

we get

$$x_1/x_2 \geqslant 1, \tag{46a}$$

the equality holding only for the exact solution. So we shall have generally either

$$x_1 \geqslant x_2 > 0$$

or

$$x_1 \leqslant x_2 < 0.$$

If f_0 corresponds to the exact solution, we shall have for the exact x:

$$x = -A_0/B_0 = -B_0/C_0$$

and

$$A_0C_0 - B_0^2 = (f_0, f_0)D_0 = 0.$$

Putting $f - f_0 = \delta f$ we find

$$\delta D = 2\begin{vmatrix} (S,C) & (S,C) & (S,f_0) \\ (S,C) & (C,C) & (C,f_0) \\ (S,\delta f) & (C,\delta f) & (f_0,\delta f) \end{vmatrix} = 0 \tag{47a}$$

$$\delta^2 D = \begin{vmatrix} (S,S) & (S,C) & (S,\delta f) \\ (S,C) & (C,C) & (C,\delta f) \\ (S,\delta f) & (C,\delta f) & (\delta f,\delta f) \end{vmatrix} > 0 \tag{47b}$$

and

$$D = D_0 + \delta D + \delta^2 D = \delta^2 D. \tag{48}$$

D_0 is stationary with respect to variations of f_0, because it is connected with $N^2 = (\omega, \omega)$ by equation (43), and therefore $\delta D = 0$. This can be seen directly by the following argument: if $\omega = S + xC + af_0$ is the exact solution then the system

$$(S,\omega) = 0, \qquad (C,\omega) = 0, \qquad (\delta f,\omega) = 0$$

is always compatible, which gives $\delta D = 0$ for any δf.

Also the determinants A, B, C can be written as

$$A = A_0+\delta A+\delta^2 A, \qquad B = B_0+\delta B+\delta^2 B, \qquad C = C_0+\delta C+\delta^2 C, \tag{49}$$

where

$$\delta A = 2\begin{vmatrix}(S,S) & (S,f_0)\\ (S,\delta f) & (f_0,\delta f)\end{vmatrix} \qquad \delta^2 A = \begin{vmatrix}(S,S) & (S,\delta f)\\ (S,\delta f) & (\delta f,\delta f)\end{vmatrix}$$

$$\delta B = \begin{vmatrix}(S,C) & (S,f_0)\\ (C,\delta f) & (f_0,\delta f)\end{vmatrix}+\begin{vmatrix}(S,C) & (S,\delta f)\\ (C,f_0) & (f_0,\delta f)\end{vmatrix} \text{ etc.} \tag{50}$$

Then from (47) we obtain

$$AC-B^2 = (A_0+\delta A+\delta^2 A)(C_0+\delta C+\delta^2 C)-(B_0+\delta B+\delta^2 B)^2 = (f_0+\delta f, f_0+\delta f)\delta^2 D,$$

from which we get

$$C_0\delta A+A_0\delta C-2B_0\delta B = 0 \tag{51a}$$

$$A_0\delta^2 C+C_0\delta^2 A-2B_0\delta^2 B+(\delta A\delta C-\delta B^2) = (f_0 f_0)\delta^2 D = (f_0 f_0)D > 0 \quad \text{etc.} \tag{51b}$$

By explicit calculations, using (50), we find

$$\delta A\delta C-\delta B^2 = -[(C,f_0)(S,\delta f)-(S,f_0)(C,\delta f)]^2 = -[(C,f_0)(S,f)-(S,f_0)(C,f)]^2 \leqslant 0, \tag{52}$$

so (51b) together with (52) yields

$$A_0\delta^2 C+C_0\delta^2 A-2B_0\delta^2 B = (f_0,f_0)D+(\delta B^2-\delta A\delta C) > 0. \tag{52a}$$

From the relation

$$x_1x_2-x^2 = \frac{A_0+\delta A+\delta^2 A}{C_0+\delta C+\delta^2 C}-\frac{A_0}{C_0} \simeq \frac{C_0\delta A-A_0\delta C+C_0\delta^2 A-A_0\delta^2 C}{C_0^2}$$

and

$$x_1-x = \frac{B_0}{C_0}-\frac{A_0+\delta A+\delta^2 A}{B_0+\delta B+\delta^2 B} \simeq \frac{B_0\delta B-C_0\delta A+B_0\delta^2 B-C_0\delta^2 A}{B_0C_0}$$

we obtain

$$C_0^2(x_1x_2-x^2)+2B_0C_0(x_1-x) \simeq 2B_0\delta^2 B-A_0\delta^2 C-C_0\delta^2 A < 0 \tag{53}$$

because of (52a). Dividing by C_0^2 we get

$$x_1x_2-x^2-2x(x_1-x) < 0$$

or

$$x^2-2x_1x+x_1x_2 < 0. \tag{54}$$

From equation (54) we find that the exact value of x lies between the values $x_1\pm[x_1(x_1-x_2)]^{1/2}$, ie

$$x_1-[x_1(x_1-x_2)]^{1/2} < x < x_1+[x_1(x_1-x_2)]^{1/2}. \tag{55}$$

We remark that as $x_1/x_2 > 1$ the expressions in (55) are always real.

In short the method is as follows: choosing a function f by parametric adjustment we make

$$N^2 = D/C \ll (S,S). \tag{56}$$

Then we calculate x_1 and x_2 and apply (55).

Usually condition (56) can be fulfilled by many sets of values of the parameters. To every one of these sets correspond generally different pairs of x_1 and x_2, and therefore we obtain various ranges for x. The overlapping of these ranges narrows the region for possible values of x, and in such way one can confine x within very close limits.

Condition (56) is necessary to preserve the inequality in deriving (54). A more detailed discussion on this point is very interesting for the applications of the method and it will be the subject of a forthcoming paper.

Since x_1 and x_2 always have the same sign the case $x \simeq 0 (x \simeq \infty)$ is easily recognized, as one finds x_1 and x_2 either positive or negative but close to (very distant from) zero.

4.2. Many-channel case

The extension to many-channel scattering is easy. Using standing waves, in the case of n channels, one has to consider a set of wavefunctions of the form:

$$\omega_i = S_i(k_i) + \sum_{j=1}^{n} x_{ij} C_j(k_j) + a_i f_i \qquad i = 1, 2, \ldots n. \tag{56}$$

Here k_i is the energy of the ith channel and $S_i(k_i)$, $C_i(k_i)$ the corresponding asymptotic expressions of the wavefunctions, similar to those of the one-channel case (see § 2.2).

The task here is to find x_{ij}'s, then using the reactance matrix technique one can derive the corresponding scattering matrix.

Without loss of generality we can take $i = 1$ and aim to calculate x_{1m}.

We form again the system:

$$\begin{aligned}
&(S_1, S_1) + \sum_{j=1}^{n} x_{1j}(S_1, C_j) + a_1(S_1, f_1) = 0 \\
&(C_i, S_1) + \sum_{j=1}^{n} x_{1j}(C_i, C_j) + a_1(C_i, f_1) = 0 \qquad i = 1, 2 \ldots n \\
&(f_1, S_1) + \sum_{j=1}^{n} x_{1j}(f_1, C_j) + a_1(f_1, f_1) = 0.
\end{aligned} \tag{57}$$

The determinant

$$D = \begin{vmatrix}
(S_1, S_1) & (S_1, C_1) \ldots (S_1, C_n) & (S_1, f_1) \\
(C_1, S_1) & (C_1, C_1) \ldots (C_1, C_n) & (C_1, f_1) \\
\vdots & \vdots \quad \vdots & \vdots \\
(C_n, S_1) & (C_n, C_1) \ldots (C_n, C_n) & (C_n, f_1) \\
(f_1, S_1) & (f_1, C_1) \ldots (f_1, C_n) & (f_1, f_1)
\end{vmatrix} \tag{58}$$

is zero only in the case of the exact solution and positive otherwise.

The only thing one has to do here, for the calculation of x_{1j}'s is to choose for each of them the 'proper' pair of systems. For example for x_{1m} one takes the following two systems: for the first we omit from system (57) the equation

$$(C_m, S_1) + \sum_{j=1}^{n} x_{1j}(C_m, C_j) + a_1(C_m, f_1) = 0$$

and for the second we omit the first equation in (57).

Then we find in an analogous way, as in the case of one channel:

$$x_{1m}^{(1)} = -A_m/B_m, \qquad x_{1m}^{(2)} = -B_m/C_m. \tag{59}$$

Again here we have

$$A_m C_m - B_m^2 = DG_m \geqslant 0 \tag{60}$$

where G_m is always positive and represents the minor determinant of D which is obtained from it if we omit the two rows and two columns which have in common the diagonal elements (S_1, S_1) and (C_m, C_m). The equality in (60) holds only in the case of the exact wavefunction.

Then we shall have also here

$$x_{1m}^{(1)}/x_{1m}^{(2)} \geqslant 1. \tag{61}$$

From now on it is clear that the procedure follows exactly the same way as in the case of one channel. Therefore we arrive at a similar condition for the bounds of x_{1m}, ie

$$x_{1m}^{(1)} - [x_{1m}^{(1)}(x_{1m}^{(1)} - x_{1m}^{(2)})]^{1/2} < x_{1m} < x_{1m}^{(1)} + [x_{1m}^{(1)}(x_{1m}^{(1)} - x_{1m}^{(2)})]^{1/2} \tag{62}$$

while the required condition is again

$$D/G_m \ll (S_1, S_1). \tag{63}$$

4.3. Numerical application

We illustrate the method with an application to $e^- H^1$ scattering in the static approximation, for $l = 0$. The Hamiltonian is reduced to its radial part which in atomic units is

$$\hat{H} = \frac{d^2}{dr^2} + k^2 + 2\left(1 + \frac{1}{r}\right) e^{-2r}.$$

We use as a trial function

$$\omega = \frac{\sin kr}{k} + \frac{x}{k}(1 - e^{-\lambda r}) \cos kr + \alpha f(r) \tag{64}$$

where

$$f(r) = r(1 + \gamma r)\, e^{-ar}. \tag{65}$$

In the application of the method the parameters λ, a and γ appear.

If we put $f_1 = r\, e^{-ar}$ and $f_2 = r^2\, e^{-ar}$ then

$$D = D_{11} + 2\gamma D_{12} + \gamma^2 D_{22} \tag{66}$$

where

$$D_{ij} = \begin{vmatrix} (S,S) & (S,C) & (S,f_i) \\ (S,C) & (C,C) & (C,f_i) \\ (S,f_j) & (C,f_j) & (f_i,f_j) \end{vmatrix} \qquad i,j = 1,2.$$

Minimizing D with respect to γ we find

$$\gamma = -D_{12}/D_{22}, \tag{67}$$

so γ is expressed in terms of the nonlinear parameters a and λ.

As the matrix elements have been calculated analytically the computing time for obtaining results for various values of the nonlinear parameters was practically negligible. The results are shown to depend very sensitively on the values of the nonlinear parameters a and λ and it was possible to find many sets of values for which the norm $N^2 = D/C$ was small in comparison with (S, S).

In table 1 we give results obtained by putting equal values for a and λ. However, there is a remarkable improvement in the results when one varies a and λ independently. This is shown in table 2 for energies $k = 0{\cdot}1$ and $k = 1$. In spite of the fact that no attempt has been made to reach the minimum of $N^2 = D/C$, the values of $N^2/(S, S)$ in all the cases of tables 1 and 2 are of the order 10^{-3}–10^{-4}.

Table 1. Bounds of phase shifts η_0. Potential $V = 2[1+(1/r)]\,e^{-2r}$, $w = 1$ and $f = r(1+\gamma r)\,e^{-ar}$.

k	$a = \lambda$	Lower bound	Upper bound	Exact†
0·1	1·5	0·70991	0·81554	0·7222
	2·8	0·62100	0·72278	
0·2	1·5	0·95704	1·03416	0·9725
	2·9	0·88430	0·97502	
0·4	2·5	1·04178	1·06518	1·0575
	2·8	1·03621	1·06374	
0·6	1·4	0·97929	1·02655	1·0210
	2·3	1·01971	1·03374	
0·8	2·4	0·96028	0·97037	0·9633
1·0	2·4	0·89375	0·90653	0·9055
	2·5	0·89953	0·94872	

† These values have been taken from a table of phase shifts, for various central potentials, computed by E J Kanellopoulos (unpublished), based on the exact solution of the Schrödinger equation (Kanellopoulos *et al* 1972).

Table 2. Bounds of phase shifts η_0. Potential $V = 2[1+(1/r)]\,e^{-2r}$, $w = 1$ and $f = r(1+\gamma r)\,e^{-ar}$.

k	a	λ	Lower bound	Upper bound	Exact
0·1	2·8	2·8	0·62100	0·72278	0·7222
	3·0	2·0	0·72112	0·72965	
1·0	2·0	2·2	0·89032	0·90568	0·9055
	2·6	1·2	0·90550	1·00813	

Appendix

The exact solution of the Schrödinger equation with a local central potential, fulfilling the conditions in § 2.1, is given (Kanellopoulos *et al* 1972) by

$$\bar{\omega} = S_l \, e^{f(r)} \Phi_1(r_{00}^{'}) + C_l \, e^{-f(r)} \int_0^r v S_l^2 \, e^{2f(r')} \Phi_1(r_{00}^{'}) \, dr' \tag{A.1}$$

where

$$f(r) = \int_0^r v S_l C_l \, dr'$$

$$\Phi_1(r_{00}^{'}) = 1 - \int_0^r v C_l^2 \, e^{-2f(r')} \, dr' \int_0^{r'} v S_l^2 \, e^{2f(r'')} \Phi_1(r_{00}^{''}) \, dr''$$

and

$$S_l = \sqrt{(\pi r/2)} J_{l+1/2}(kr), \qquad C_l = \sqrt{(\pi r/2)} Y_{l+1/2}(kr).$$

Taking

$$\omega = \bar{\omega} / e^{f(\infty)} \Phi_1(\infty_{00})$$

and

$$x = \frac{e^{-2f(\infty)} \int_0^\infty v(r) S_l^2 \, e^{2f(r)} \Phi_1(r_{00}^{'}) \, dr}{\Phi_1(\infty_{00})}.$$

we can write

$$\omega = S_l + x C_l g + S_l \left(\frac{e^{f(r)} \Phi_1(r_{00}^{'})}{e^{f(\infty)} \Phi_1(\infty_{00})} - 1 \right) + x C_l \left(\frac{e^{-f(r)} \int_0^r v S_l^2 \, e^{2f(r')} \Phi_1(r_{00}^{'}) \, dr'}{e^{-f(\infty)} \int_0^\infty v S_l^2 \, e^{2f(r)} \Phi_1(r_{00}^{'}) \, dr} - g(r) \right). \tag{A.2}$$

Comparing this with (9) we see that Φ is the sum of the last two terms on the right-hand side of (A.2). It is now quite simple to show that each of these terms is normalizable provided that $v(r)$ and $dg(r)/dr$ fall at infinity faster than $r^{-3/2}$.

References

Feshbach H and Rubinow S 1952 *Phys. Rev.* **88** 484–7
Harris F E 1967 *Phys. Rev. Lett.* **19** 173–5
Harris F E and Michels H H 1967b *Phys. Rev. Lett.* **19** 885–6
—— 1969 *Phys. Rev. Lett.* **22** 1036–9
Hulthén L 1944 *K. Fysiograf. Sällsk. Lund Förh.* **14** No 21 257
—— 1948 *Ark. Math. Astron. Fys.* **35A** 25
Hulthén L and Skavlem S 1952 *Phys. Rev.* **87** 297–303
Kanellopoulos E J, Kanellopoulos T V and Wildermuth K 1972 *Comm. Math. Phys.* **24** 233–42
Kato T 1951 *Prog. Theor. Phys.* **6** 394–407
Kohn W 1948 *Phys. Rev.* **74** 1763–71
Ladányi K and Szondy T 1971 *Nuovo Cim.* B **5** 70–8
Nesbet R K 1968 *Phys. Rev.* **175** 134–42
—— 1968 *Phys. Rev.* **179** 60–70
Spruch L and Rosenberg L 1960 *Phys. Rev.* **117** 143–51
Schmid E W and Schwager J 1972 *Nucl. Phys.* A **180** 434–48
Schwartz C 1961 *Ann. Phys., NY* **16** 36–50