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Bounds on Multichannel Scattering Parameters*

YUKAP HAHN, THOMAS F. O'MALLEY,† AND LARRY SPRUCH
Physics Department, New York University, Washington Square, New York, New York

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Using the projection techniques recently developed in the formal theory of reactions, it is shown that a bound on the exact reactance matrix K is provided by the close-coupling reactance-matrix approximation K^P; that is, K-K^P is, in a sense that can be made precise, a positive definite operator. This is of more than formal interest since the numerical solution of the finite number of coupled equations which arise when we allow the target system to be excited to only a restricted number of virtual states, and the determination of K^P is feasible for a variety of three-body problems which includes, of course, three-body model problems. Furthermore, K^P improves monotonically as one includes more and more virtual states. The recognition of this monotonicity property is useful in self-consistency analyses during the course of numerical calculations, and provides a more precise meaning for the numerical results obtained. Choosing a particular representation, the bound on K generates bounds on the appropriately defined eigenphase shifts. The question of the absolute definition of phase shifts and of eigenphase shifts is discussed in some detail and it is shown that the presently used definition has serious deficiencies.

1. INTRODUCTION

IN the minimum-principle formulation of scattering theory,[1-4] an expression containing an arbitrary number of variational parameters is shown to represent an upper bound on the scattering parameter under consideration. The situation is then analogous to that which obtains in the Rayleigh-Ritz evaluation of the ground-state energy of a system. The introduction of more and more parameters enables one systematically to approach the true result monotonically and, at least in principle, to come arbitrarily close to it.

An altered minimum-principle formulation was recently given[4] which, for single-channel scattering at nonzero energies, represents a significant improvement upon the earlier version. The improvement is a consequence of the utilization of recent developments in the formal theory of scattering due largely to Feshbach,[5,6] which, as opposed to the Wigner-Eisenbud formalism, does not require any of the potentials to be truncated. The newer version of the minimum-principle formulation has been extended to the multichannel scattering and will be reported on shortly. It has also been shown, for single-channel scattering, that various close-coupling approximations in common use provide a bound on the true phase shift.[7,8] (This bound is a number; it contains no variational parameters. In our earlier papers, when we were primarily concerned with the minimum principle, we unfortunately did not distinguish between the words minimum principle and bound.) The present paper will be largely concerned with the extension of the phase-shifts bound of Ref. 7 to multichannel scatterings, that is, to the determination of a bound on the reactance matrix K which characterizes multichannel scattering. The multichannel scattering process is, of course, determined by the specification of the eigenphase shifts and of the mixing parameters.

Physical effects are, of course, never affected by changes of multiples of 2π in phase shifts or in eigenphase shifts, and they are often not affected by changes of odd multiples of π. It should therefore be clear that one cannot argue on physical grounds that the phase shifts or eigenphase shifts must be continuous in any parameter, but rather one must allow for jumps of 2π or perhaps π, and we will find instances in which a perfectly sensible definition of the shifts leads to shifts which are discontinuous by 2π or π in, for example, the energy. It is nevertheless often useful to impose some restrictions on the multiples of π; we will cite some examples shortly. One possibility is to fix the multiples of π absolutely, in which case one has an absolute definition of the phase shifts and eigenphase shifts. Another possibility is to impose the condition that the shifts be continuous in some parameter, such as the energy, in which case the difference in the shifts for two different values of the parameter is fixed.

We will cite just three examples where useful results can be obtained by imposing certain requirements on the phase shifts, that is, where something more than just the phase shifts modulo 2π is of physical interest

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† Presently visiting fellow, Joint Institute for Laboratory Astrophysics, Boulder, Colorado.

[1] L. Spruch and L. Rosenberg, Phys. Rev. **116**, 1034 (1959); and **117**, 1095 (1960); L. Rosenberg, L. Spruch, and T. O'Malley, *ibid.* **118**, 184 (1960).

[2] L. Rosenberg and L. Spruch, Phys. Rev. **121**, 1720 (1961); and **125**, 1407 (1962).

[3] A review of the various papers that develop the theory, including the above, and of the applications, is given by L. Spruch in *Lectures in Theoretical Physics*, edited by W. E. Brittin, W. B. Downs, and J. Downs (Interscience Publishers, Inc., New York, 1963), Vol. 4.

[4] Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. **130**, 381 (1963).

[5] H. Feshbach, Ann. Phys. (N. Y.) **5**, 357 (1958).

[6] See also L. Fonda and R. G. Newton, Ann. Phys. (N. Y.) **10**, 490 (1960).

[7] Y. Hahn, T. O'Malley, and L. Spruch, Phys. Rev. **128**, 932 (1962).

[8] See also I. C. Percival, Phys. Rev. **119**, 159 (1960).

even though no measurable quantity is affected. The three examples are all concerned with the simple case of scattering by a static central local potential. We are then of course dealing only with phase shifts, and not with eigenphase shifts.

(i) We demand that $\eta(E)$, the phase shift for angular momentum L at the energy E, be continuous in E. That is, we reject the physically allowable possibility of arbitrarily adding different multiples of π to η at different energies. (We have not, however, given an absolute definition of η.) We then have Levinson's theorem, that

$$\eta(E=0)-\eta(E=\infty)=N\pi\,,$$

where N is the number of bound states of angular momentum L. Note that N also represents the number of nodes other than that at the origin of the zero-energy scattering wave for angular momentum L.

(ii) The question of the convergence of the Born expansion is connected with the absolute value of η. (In this and the following example, it is possible to replace the requirement of an absolute definition of η by a continuity requirement.)

(iii) Take any of the usual absolute definitions of η. (These will be quoted shortly.) Then if $V(r)\leq 0$ for all r, and if η is less than $\frac{1}{2}\pi$, the Lippmann-Schwinger Green's function variational principle for $k\cot\eta$ provides an upper bound on the exact value of $k\cot\eta$ for an arbitrary trial function.[9] A corresponding statement can be made if $V(r)\geq 0$ for all r. As one small corollary of this result, it follows[10] if $V(r)\leq 0$ for all r, if $\eta_+<\frac{1}{2}\pi$, and if $\eta_->-\frac{1}{2}\pi$, where η_+ and η_- are the phase shifts associated with $V(r)$ and $-V(r)$, respectively, that

$$\cot\eta_+-\cot\eta_-\leq 2\cot\eta_{B+}\,,$$

where η_{B+} is the Born-approximation phase shift associated with $V(r)$.

Let us now briefly consider the scattering of a particle by a compound system. Even for single-channel (elastic) scattering, it is not at all clear how best to define an absolute phase shift. We will in fact show that the definition that appears in the literature,[2,11] while allowable, is inconsistent with and for most purposes less useful than a number of other possible definitions. It will therefore be necessary to reexamine the results obtained in the paper on the bounds on single-channel phase shifts.[7] We will at the same time, and this will in fact be our main purpose, extend the energy domain of applicability of the results of that paper to include energies above resonance but below the threshold for excitation, and generalize the results to include multichannel scattering. The emphasis throughout will be on numerical results related to close-coupling approximation calculations, that is, to calculations in which one solves exactly the approximate problem in which all open channels and a prescribed set of (virtually excited) closed channels are taken into account.[12] The results to be obtained will be useful during the course of numerical calculations by providing self-consistent checks on the numerical results. Our results will also allow for a more precise interpretation of the meaning of the numerical results obtained in such approximate calculations.

We will have a few comments to make on the absolute definition of phase shifts and of eigenphase shifts, but primarily we will be concerned with variations in the shifts with respect to some parameters. The formalism as presented is not applicable to systems in which there are open channels with three or more particles or systems at arbitrarily large separation, and there is then an upper limit to the energy that we can consider. We will not therefore be concerned with extensions of Levinson's theorem to scattering by a compound system.

2. DEFINITION OF PHASE SHIFT FOR SINGLE-CHANNEL SCATTERING

We will consider, in order, scattering by a central static local potential, and scattering by a central static nonlocal potential. [The latter is a particular but simple example of elastic (single-channel) scattering by a compound system.] The discussion will be somewhat detailed since there has been a good deal of confusion in the literature.

The phase shift for scattering by a central static local potential is a function of the energy of the incident particle, which for simplicity we take to be spinless and uncharged, and of the strength of the potential. Two absolute definitions of the phase shift are thereby suggested.

(1) Define η to be zero for infinite incident energy and to be a continuous function of the energy.

(2) Replace the true potential $V(r)$ by $\lambda V(r)$, introduce the associated phase shift $\eta(\lambda)$ with $\eta=\eta(1)$, set $\eta(0)=0$, and take $\eta(\lambda)$ to be continuous in λ.

It will almost always also be possible to define η by considering variations in the effective range of the potential and, having gone over to the radial equation, by considering variations in the angular momentum, but we will not consider these two possibilities.

There are two other absolute definitions of η which are in some ways more appealing than those just recorded. In an actual numerical calculation one after all keeps the energy, the angular momentum, and the potential fixed, and determines the scattering wave function, and it would therefore be nice to have an absolute definition of η which required only a knowledge of the scattering wave function for the energy, angular momentum, and potential of interest. This suggests the following two definitions:

(3) Replace $V(r)$ by $V(r)\Sigma(r-R)$, where $\Sigma(\epsilon)=1$ for

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[9] T. Kato, Phys. Rev. **80**, 475 (1950).

[10] L. Spruch, Phys. Rev. **109**, 2149 (1958).

[11] A. Temkin, J. Math. Phys. **2**, 336 (1961).

[12] A review of the theory and of some of the applications of the close-coupling approximation is contained in P. G. Burke and K. Smith, Rev. Mod. Phys. **34**, 458 (1962).

$\epsilon > 0$ and $\Sigma(\epsilon) = 0$ for $\epsilon < 0$, introduce the associated phase shift $\eta(R)$ with $\eta = \eta(0)$, set $\eta(\infty) = 0$, and take $\eta(R)$ to be continuous in R. It should be remarked that on integrating out numerically from the origin, the logarithmic derivative of the wave function at $r = R$ is unaffected by the potential still to be felt, so that $\eta(R)$ has a perfectly well-defined meaning. One integrates out numerically from the origin once and only once, and the scattering wave function thereby obtained determines $\eta(R)$ for all R.[13]

(4) Let $r^{(m)}$ and $\rho^{(m)}$ be the positions of the mth node of the true scattering wave function and of the free-wave scattering function, $krj_L(kr)$, respectively, and define η by

$$\eta \equiv \lim_{m\to\infty} \pi(\rho^{(m)} - r^{(m)}).$$

This definition will be referred to as the nodal definition of η.

Now we will not prove it, but the four different absolute definitions of η that have been given are entirely equivalent. Thus, for $E = \infty$, for $\lambda = 0$, *or* for $R = \infty$, the exact scattering wave function is the free scattering wave function, for which the nodal definition gives $\eta = 0$. [Some care must be exercised in studying the limit $E \to \infty$ if $V(r)$ has a $1/r$ singularity at the origin.] The various definitions therefore all agree with the nodal definition for the given value of the parameter, that is, for $E = \infty$, $\lambda = 0$, or $R = \infty$. We now state without proof, though it is the crucial point in the argument, that the nodal definition gives rise to an η which, for the static local central potential under consideration, is continuous in E, in λ, and in R. It follows that the various definitions agree with the nodal definition for the parameter of interest, namely the given energy, $\lambda = 1$, or $R = 0$. Since the various definitions all agree with a given definition, the nodal definition, they are clearly entirely equivalent for the local static central potential under consideration.

We now consider scattering by a nonlocal potential, and show that as contrasted with the local potential case the four definitions of η given above are *not* necessarily all equivalent. This distinction between local and nonlocal interactions has its origin in the fact that the wave function and its derivative can vanish at the same point for a nonlocal, but not for a local interaction.

The lack of the equivalence of the four definitions of η for nonlocal potentials can arise in a wide variety of cases, and is in no sense restricted to pathologic cases such as that for which there is a bound state embedded in the continuum. Consider, for example, the case of a nonlocal interaction which is separable, the kernel being $\lambda f(r) f(r')$. For simplicity we take $L = 0$. This is a solvable problem with the wave function to be called $v(\lambda, r)$ given by

$$v(\lambda,r) = \sin kr - \lambda C \int_0^\infty dr' G(r,r') f(r'),$$

where

$$C = \int_0^\infty dr' f(r') \sin kr' \Big/ \left[1 + \lambda \int_0^\infty dr \int_0^\infty dr' G(r,r') f(r) f(r')\right],$$

and where

$$G(r,r') = (1/k) \sin kr_< \cos kr_>$$

is the free-particle Green's function. By construction we have $v(\lambda, 0) = 0$, and we also have

$$v'(\lambda,0) = k - \lambda C \int_0^\infty dr' f(r') \cos kr'.$$

It is then clear that for any energy E there will be one value of λ, to be called $\lambda(E)$, for which $v(\lambda, r)$ *and* its derivative vanish at the origin. The number of nodes of $v(\lambda, r)$ is not then a continuous function of λ, but jumps by 1 as one passes through $\lambda = \lambda(E)$. It follows that one can define η by (2) *or* by (4), but that the two definitions need not be consistent.

One can also find nonlocal potentials for which $v(\lambda, r)$ and its derivative both vanish at some point other than the origin; the number of nodes of $v(\lambda, r)$ as a function of λ will then jump by 2 at the appropriate value of λ. More significantly, by considering energy-dependent separable nonlocal potentials with kernels

$$[\lambda/(E - E_0)] f(r) f(r'),$$

it is simple to show that continuity of η in λ can be incompatible with continuity of η in E, that is, definitions (1) and (2) can be incompatible.[14]

We are now in a position to analyze the definition of η that has been given[2,11] for the scattering of a particle by a compound system under circumstances such that elastic scattering is the only allowable process. To begin with, we must recall that none of the four definitions of η given above can be extended in any obvious way, if indeed in any way at all, to the general elastic scattering process. Thus, if we attempt to use definition (1) we cannot go to $E = \infty$ without passing out of the domain of single-channel scattering. If we are dealing with identical particles, we cannot always use definition (2). For the scattering of electrons by hydrogen atoms, for example, any change of the strength of the incident electron-proton interaction requires that we change the bound electron-proton interaction and hence the ground state of the target; if we change only the strength of the electron-electron interaction, the incident electron will start to see a net charge on the target, with ensuing complications. Definition (3) suffers from the same defect for if we cut off the interaction of the incident particle with the target we may have to cut off the interactions of the particles within the target. This defini-

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[13] F. Calogero, Nuovo Cimento **27**, 261 (1963).

[14] R. G. Newton, Ann. Phys. (N. Y.) 4, 29 (1958).

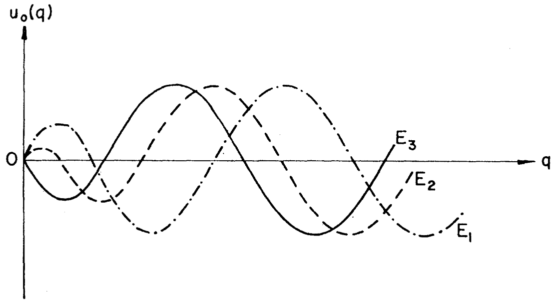

FIG. 1. The projected wave function $u_0(q)$ for the energies E_1, E_2, and E_3.

tion also loses the advantage that it had over definitions (1) and (2) for scattering by a local potential, for now one would have to redo the calculation for each value of R since the wave function for $r<R$ *is* now affected in more than its normalization by the potential that exists beyond $r=R$. Definition (4) may now be ambiguous, for we would have to fix the target coordinates if we are to reduce the scattering wave function to a function of one coordinate, and the number of nodes of the one-coordinate function could depend upon precisely how the target coordinates are fixed. The definition that was given[2,11] involved the introduction of an equivalent one-body problem. Letting q represent the distance between the incident particle and the center of mass of the target, the function $u_0(q)$ defined as the radial part of the projection of the full scattering function onto the ground-state wave function of the target was introduced. Since the one-body function $u_0(q)$ could easily be seen to satisfy the usual boundary conditions of a scattering function, $u_0(q)$ was then a function that would arise in some potential scattering problem. An application of the nodal definition to $u_0(q)$ might then seem to lead to a natural definition of the phase shift. It is important to observe, however, that the equivalent one-body problem of which $u_0(q)$ is the solution is that for which the potential is the optical-model potential, which is an energy-dependent nonlocal interaction. [See Eqs. (22) and (23).] While the above definition is permissible, the four definitions of η are not then necessarily equivalent, and the assumption that they are can lead, if used in the interpolation of numerical calculations, to physically incorrect predictions.

Assume, for example, that we are studying elastic scattering in an energy region in which the phase shift is a rapidly varying function of the energy. The numerical calculations may well then be particularly difficult to perform especially if one is using an iterative procedure, and it would be very convenient to be able to minimize the number of values of the energy at which the calculation is to be performed, and to determine η at intermediate energies by continuity arguments. Now let us assume that the (presumably accurate) projected wave function, $u_0(q)$, determined at the energies E_1, E_2, and E_3, where $E_1<E_2<E_3$, has the form given in Fig. 1, the number of nodes of $u_0(q)$ having decreased by one at some energy between E_2 and E_3. If η is taken to be continuous in E, the appropriate curve in Fig. 2 is abcdef. If, on the contrary, one defines the phase shift in terms of the number of nodes of $u_0(q)$, the appropriate curve is the discontinuous curve abcdd′e′f′. The two curves lead to identical physical predictions. If, however, one were to apply the nodal definition to $u_0(q)$ to fix η at b, c, and e′ at the energies E_1, E_2, and E_3, respectively, *and* to assume that η is continuous in the energy, one would arrive at a curve of the form abce′f′, following something like the dashed curve between c and e′, and the predicted cross section would be physically incorrect.[15]

The realization that the various definitions of η are not necessarily compatible also requires some reinterpretation of the conclusions reached in the paper on bounds on the phase shift for single-channel scattering.[7] We will discuss this point below in the broader context of multichannel scattering processes.

3. CLOSE-COUPLING APPROXIMATIONS AND BOUNDS ON THE *K* MATRIX

A standard approximation in the study of the scattering of a particle by a compound system when there are N open channels is the close-coupling approximation. One does a partial-wave decomposition and then approximates the true solution Ψ by a function of the form

$$\Psi^P=\Sigma'\psi_{Tm}(\mathbf{r})u_m{}^P(\mathbf{q}), \qquad (1)$$

appropriately antisymmetrized, where $\psi_{Tm}(\mathbf{r})$ represents the wave function for the mth state of the target system, with associated energy E_{Tm}, and where the $M(\geq N)$ terms in the (restricted) sum include all possible final states of the target, that is, all N open

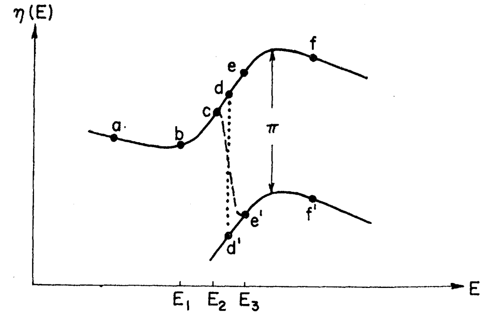

FIG. 2. The phase shift as a function of the energy. The assumption that η is determined by the number of nodes in $u_0(q)$ *and* that η is continuous in the energy leads to the incorrect curve *abce′f′*, with something approximating the dashed curve between *c* and *e′*.

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[15] The situation just described is precisely that which occurred in a recent approximate numerical analysis of the scattering of electrons of zero angular momentum at energies in the neighborhood of a resonance, just below the threshold for excitation. At our suggestion an additional calculation was performed at an energy between E_2 and E_3 and the numerical value found was indeed different from that which had originally been predicted. See A. Temkin and R. Pohle, Phys. Rev. Letters **10**, 22 (1963); and **10**, 268 (1963).

channels, and $M-N$ closed channels. If we demand that

$$\int \psi_{Tm}(\mathbf{r})(H-E)\Psi^P(\mathbf{r},\mathbf{q})d\mathbf{r}=0 \tag{2}$$

for each of the values of m included in the sum, we are led to the set of M coupled equations

$$P(H-E)P\Psi^P=0\,, \tag{3}$$

where P is the projection operator onto the set of M states. The (numerical) solution of these equations, that is, the determination of the $u_m{}^P(\mathbf{q})$, leads to an approximation K^P for the N by N reactance matrix K. It will be the purpose of this section to prove that K^P provides a bound on K.

The proof will be a generalization to multichannel scattering of that given in our earlier paper on single-channel scattering.[7] The proof will, however, represent an improvement as well as a generalization for we will remove the restriction there imposed to energies up to the first resonance; the present proof will be valid up to the threshold energy for the opening up of a new channel. On the other hand, in connection with our discussion of the previous section on the absolute definition of the phase shift, the results there obtained will be seen to be not quite as strong as we had believed them to be.

Though the results can be obtained under quite general conditions, we will for simplicity assume that the various spins are zero and that there are no net Coulombic fields. We will also assume that all of the open channels are two-system channels; this latter assumption is required for the present approach and is not just a matter of simplicity. We introduce the projection operator Q which projects onto all of the states not included in the primed sum. We then have $Q=1-P$ and $PQ=0$. We are interested in numerical results, and if the formalism to be developed is to have any content it must be possible to give an explicit and usable form for P. This can be done for a variety of interesting cases.

The approach is the same as that for single-channel scattering.[7] With the indices i and j referring to open channels only, we write

$$(H-E)\Psi=0 \tag{4}$$

as

$$P(H-E)P\Psi=-PHQ\Psi\,, \tag{5}$$

$$Q(H-E)Q\Psi=-QHP\Psi\,. \tag{6}$$

$P\Psi$ is now an M-component wave function which must be regular at the origin and which must have the asymptotic form in the ith (open) channel:

$$P\Psi \rightarrow D_i\psi_{Ti}(\mathbf{r})(a_is_{i\theta}+b_{i\theta}c_{i\theta})/q_i\,, \tag{7}$$

where

$$s_{i\theta}=\sin(k_iq_i-\tfrac{1}{2}L_i\pi+\theta)\,, \tag{8}$$

$$c_{i\theta}=\cos(k_iq_i-\tfrac{1}{2}L_i\pi+\theta)\,, \tag{9}$$

$$(k_i^2\hbar^2/2\mu_i)+E_{Ti}=(k^2\hbar^2/2\mu_0)+E_{T0}\,. \tag{10}$$

μ_i is the reduced mass and L_i is the relative orbital angular momentum quantum number for channel i. D_i contains the factor $(\mu_i/k_i)^{1/2}$, spherical harmonics in $\mathbf{q}_i/q_i$, and the Clebsch-Gordon coefficients necessary to give the prescribed value of the total angular momentum. θ is a parameter to be chosen for convenience,[16] subject to the requirement that $0\leq\theta<2\pi$. The a_i are arbitrary constants and the $b_{i\theta}$ are to be determined. The vectors constructed from the numbers a_i and $b_{i\theta}$ will be denoted by $\mathbf{a}$ and $\mathbf{b}_\theta$, respectively. The a_i and the $b_{i\theta}$ are connected by the relationship

$$b_{i\theta}=\sum_j{}' K_{\theta ij}a_j\,, \tag{11}$$

where as indicated by the index the sum is over open channels. The connection between the matrix $\mathbf{K}_\theta$ and the usual reactance matrix $\mathbf{K}$ is given by

$$\mathbf{K}_\theta=\frac{-\sin\theta\mathbf{1}+\cos\theta\mathbf{K}}{\cos\theta\mathbf{1}+\sin\theta\mathbf{K}}\,, \tag{12}$$

where $\mathbf{1}$ is the unit matrix. $Q\Psi$ is regular at the origin and since it contains only closed channels it decays more rapidly than the inverse of the relative coordinate for each of its (closed) channels. The formal solution of Eq. (5) is

$$P\Psi=P\Psi^P+G^PPHQ\Psi\,, \tag{13}$$

where

$$G^P\equiv[P(E-H)P]^{-1} \tag{14}$$

is the $M\times M$ matrix which connects the M channels under consideration. $P\Psi^P$ is that solution of Eq. (3) which is regular at the origin and which behaves in the ith channel as

$$P\Psi^P\rightarrow D_i\psi_{Ti}(a_is_{i\theta}+b_{i\theta}{}^Pc_{i\theta})/q_i\,,\quad q_i\rightarrow\infty\,. \tag{15}$$

The M coupled equations which, with the prescribed boundary conditions, determine $P\Psi^P$ must be solved exactly. G^P is clearly not uniquely determined by Eq. (14). To make it unique we note that it follows from Eqs. (7) and (13) that in the ith (open) channel

$$G^PPHQ\Psi\rightarrow D_i\psi_{Ti}(b_{i\theta}-b_{i\theta}{}^P)c_{i\theta}/q_i\,,\quad q_i\rightarrow\infty\,. \tag{16}$$

G^P is then made unique by demanding that $G^PPHQ\Psi$ not contain any $s_{i\theta}$ components.

The formal solution of Eq. (6) is given by

$$Q\Psi=G^QQHP\Psi\,, \tag{17}$$

where

$$G^Q\equiv[Q(E-H)Q]^{-1}. \tag{18}$$

If there are any solutions of the homogeneous equations associated with Eq. (6), with energies $\mathcal{E}_n{}^Q$, the effective one-body potential for the incident particle is infinite at $E=\mathcal{E}_n{}^Q$, since G^Q is infinite at that energy. [See Eq. (19).] We will see that no difficulties are occasioned

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[16] It is possible to choose a different value of θ for each channel, as was done in the second paper in Ref. 2, but we will not do so. It then seemed to be a useful device since it allowed one to choose different truncation radii for the different channels, but we are no longer truncating the potentials.

by this occurrence, a fact which is perhaps made more reasonable by the remark that it is a *nonlocal* potential which is passing through infinity. It should also be noted that the $\mathcal{E}_n{}^Q$ are not the resonance energies, but differ from them by the usual energy shift. We also remark that as opposed to G^P, the expression for G^Q, Eq. (18), is a purely formal one; Q projects onto an infinite-dimensional space, and one cannot obtain an expression for G^Q with which one can actually perform numerical calculations. Substitution of Eq. (17) into the right-hand side of Eq. (5) leads to a homogeneous equation for $P\Psi$,

$$P[H+HQG^QQH-E]P\Psi=0\,, \tag{19}$$

while substitution of Eq. (13) into the right-hand side of Eq. (6) leads to an inhomogeneous equation for $Q\Psi$,

$$Q[H+HPG^PPH-E]Q\Psi=-QHP\Psi^P. \tag{20}$$

Each of these equations is formally equivalent to the original Schrödinger equation, since a knowledge of $P\Psi$ determines $Q\Psi$ and vice versa by Eqs. (17) and (13), respectively. As for single-channel scattering, Eq. (19) will be used for the determination of a *bound* on $\mathbf{K}_\theta$ while Eq. (20) will be used as the starting point for the development of a *minimum principle* for $\mathbf{K}_\theta$ in a paper to be submitted shortly.

Now H is given by

$$H(\mathbf{r},\mathbf{q})=H_T(\mathbf{r})+T(\mathbf{q})+V(\mathbf{r},\mathbf{q})\,, \tag{21}$$

where H_T is the target Hamiltonian with $\mathbf{r}$ all of the target coordinates, $T(\mathbf{q})$ is the kinetic energy operator of the incident particle, and $V(\mathbf{r},\mathbf{q})$ is the interaction of the incident particle with the target. (For simplicity, the arguments will be given for distinguishable particles, but it can be extended to indistinguishable particles.) Eq. (19) can be written as

$$[T(\mathbf{q})\mathbf{1}+\mathcal{V}(\mathbf{q})-(E\mathbf{1}-\mathbf{E}_T)]\mathbf{u}(\mathbf{q})=0\,, \tag{22}$$

where $\mathbf{1}$ is the $M\times M$ unit matrix, $\mathbf{E}_T$ is the diagonal matrix with diagonal elements E_{Tm} and $\mathbf{u}(\mathbf{q})$ is the column vector with elements $u_m(\mathbf{q})$. The (optical-model) $M\times M$ matrix potential $\mathcal{V}(\mathbf{q})$ is given by

$$\mathcal{V}(\mathbf{q})=\int d\mathbf{r}\psi_T(\mathbf{r}) \times\left[V+VQ\frac{1}{Q(E-H_T-T)-QVQ}QV\right]\psi_T{}^\dagger(\mathbf{r})\,, \tag{23}$$

where $\psi_T(\mathbf{r})$ is a column vector with elements ψ_{Tm}, and where we have used the fact that Q commutes with $H_T(\mathbf{r})$ and with $T(\mathbf{q})$. On introducing the $M\times M$ matrix $\mathcal{V}(\mathbf{q},\lambda)$ (see Appendix),

$$\mathcal{V}(\mathbf{q},\lambda)=\int d\mathbf{r}\psi_T(\mathbf{r}) \times\left[V+\lambda VQ\frac{1}{Q(E-H_T-T)-\lambda QVQ}QV\right]\psi_T{}^\dagger(\mathbf{r})\,, \tag{24}$$

we have

$$\mathcal{V}(\mathbf{q})=\mathcal{V}(\mathbf{q},1)\,. \tag{25}$$

Since

$$\frac{d}{d\lambda}\frac{1}{A-\lambda B}=\frac{1}{A-\lambda B}B\frac{1}{A-\lambda B} \tag{26}$$

if the operators A and B are independent of λ,

$$\frac{d}{d\lambda}\mathcal{V}(\mathbf{q},\lambda)=\chi Q(E-H_T-T)Q\chi^\dagger\,, \tag{27}$$

where

$$\chi=\frac{1}{Q(E-H_T-T-\lambda V)Q}QV\psi_T\,. \tag{28}$$

Since Q projects onto closed channels only, it follows that $Q(E-H_T-T)Q$ and therefore that $d\mathcal{V}(\mathbf{q},\lambda)/d\lambda$ are negative definite operators.

Consider now the equation

$$[T(\mathbf{q})\mathbf{1}+\mathcal{V}(\mathbf{q},\lambda)-(E\mathbf{1}-\mathbf{E}_T)]\mathbf{u}(\mathbf{q},\lambda)=0\,, \tag{29}$$

and the corresponding equation with λ replaced by $\lambda+d\lambda$; multiply the equation for $\mathbf{u}(\mathbf{q},\lambda)$ by $\mathbf{u}^\dagger(\mathbf{q},\lambda+d\lambda)$ and the equation for $\mathbf{u}(\mathbf{q},\lambda+d\lambda)$ by $\mathbf{u}^\dagger(\mathbf{q},\lambda)$, subtract and integrate. With $\mathbf{K}_\theta(\lambda)$, the reactance matrix associated with $\mathcal{V}(\mathbf{q},\lambda)$, one then arrives at

$$\frac{d}{d\lambda}(\mathbf{a}\cdot\mathbf{K}_\theta(\lambda)\mathbf{a})=-\int d\mathbf{q}\mathbf{u}^\dagger(\mathbf{q},\lambda)\left[\frac{d}{d\lambda}\mathcal{V}(\mathbf{q},\lambda)\right]\mathbf{u}(\mathbf{q},\lambda)\,, \tag{30}$$

and the inequality then follows from the negative definiteness of $d\mathcal{V}(\mathbf{q},\lambda)/d\lambda$. Since a is normalized but otherwise arbitrary, $d\mathbf{K}_\theta(\lambda)/d\lambda$ is a positive definite operator, that is, that

$$d\mathbf{K}_\theta(\lambda)/d\lambda\geq 0\,. \tag{31}$$

More precisely, the derivative is positive definite where it exists, for since the denominator in Eq. (28) for χ can be equal to zero, χ and therefore $d\mathcal{V}(\mathbf{q},\lambda)/d\lambda$ and hence $d\mathbf{K}_\theta(\lambda)/d\lambda$ and finally $\mathbf{K}_\theta(\lambda)$ itself can be infinite.

To understand the consequence of Eq. (31), let us first consider the special case of single-channel scattering. Since $\mathbf{K}_\theta(\lambda)$ for single-channel scattering is $\tan[\eta(\lambda)-\theta]$, Eq. (31) then reduces to

$$\frac{d}{d\lambda}\tan[\eta(\lambda)-\theta)]=\sec^2[\eta(\lambda)-\theta)]\frac{d\eta(\lambda)}{d\lambda}\geq 0\,. \tag{32}$$

Now $\mathbf{K}_\theta(\lambda)$ is a uniquely defined quantity, but as always there is an arbitrariness in the value of η. We will for the moment only partially remove this arbitrariness. With the multiples of π in the definition of $\eta(\lambda=0)$ unspecified, we impose the requirement that $\eta(\lambda)$ be continuous in λ as λ varies from zero to one, even if $\mathbf{K}_\theta(\lambda)$ passes through infinity. The introduction of a phase shift is equivalent to keeping track of which branch of $\mathbf{K}_\theta(\lambda)$ we are on, that is, how many times $\mathbf{K}_\theta(\lambda)$ has passed through infinity. Our final conclusion is that

$$\eta(\lambda=0)=\eta^P<\eta\,. \tag{33}$$

It is simple to obtain a slight generalization of Eq. (31). P is defined as before, but Q will be redefined. Consider a projection operator $P^\star$ which projects onto all of the states projected onto by P and onto some additional states, with a corresponding wave function $\Psi^{P^\star}$ and matrix $K^{P^\star}$. We again have P and Q as projection operators, but now $P+Q$ is not defined as spanning the entire space but just $P^\star$ space—$P^\star$ can of course be the unit operator and span all of space—so that $P^2=P$, $Q^2=Q$, $P+Q=P^\star$, $P^{\star 2}=P^\star$, and $PQ=0$. Our starting point is now

$$P^\star(H-E)P^\star\Psi^{P^\star}=0\,, \tag{34}$$

and all of the equations derived above in this section are valid under the replacements $\Psi\rightarrow\Psi^{P^\star}$, $\eta\rightarrow\eta^{P^\star}$, $K_\theta\rightarrow K_\theta{}^{P^\star}$, and with Q no longer equal to $1-P$ but reinterpreted as $Q=P^\star-P$. Eq. (31) is now to be understood as meaning that $\mathbf{K}_\theta{}^P(\lambda)$, where it exists, is a monotonically increasing function of λ. Now as λ varies between 0 and 1, we pass from P space to $P+Q=P^\star$ space. For single-channel scattering, we then have

$$\eta^P\leq\eta^{P^\star}. \tag{35}$$

Since Eq. (33) becomes, on the replacement of P by $P^\star$, $\eta^{P^\star}\leq\eta$, we have

$$\eta^P\leq\eta^{P^\star}\leq\eta. \tag{36}$$

Consider for example the (elastic) scattering of electrons by hydrogen atoms, with the Pauli principle taken into account, for energies up to $\frac{3}{4}\times13.6$ eV, the threshold for excitation. We then have

$$\eta(1s)\leq\eta(1s+2s)\leq\eta(1s+2s+2p)\leq\cdots\leq\eta\,, \tag{37}$$

where the argument indicates the target states included. These inequalities are also valid for the (elastic) scattering of positrons by hydrogenic atoms for energies up to the pickup threshold, 6.8 eV.

In spite of the existence of the inequalities given by (36), and contrary to the claim in our previous paper, one can never assert with complete certainty from a study of a sequence of numerical calculations in which more and more target states are added, that any numerical result is in error. [We incorrectly presumed in that paper that one could define η in terms of the nodes in $u_0(q)$ *and* that one could demand that η be continuous in λ.] The numerical calculations after all only give the phase shifts modulo π, and inequalities of the form (36) can always be satisfied by adjustment of the multiples of π. The realization that such inequalities exist can nevertheless be very helpful. If, for example, one believes that the space spanned by P is large enough to include all of the very significant hydrogenic states, one would be rather sure that the inclusion of an additional state would have little influence on the phase shift and in particular would not change the phase shift by anything comparable with π. Since, by assumption, the states projected onto by $P^\star$ include all of the states projected onto by P, one would therefore predict firstly that one can then adjust $\eta^{P^\star}$ by adjusting the multiples of π so that $\eta^{P^\star}$ will be quite close to η^P, and secondly that $\eta^{P^\star}$ so chosen will be slightly greater than η^P. In the analysis[7] of the numerical calculations for the elastic scattering of electrons by hydrogen atoms, there was a total of over 30 predictions of relative magnitude of phase shifts calculated in different approximations; all but one of these was satisfied, and even in the light of our realization of incompatibility of the different definitions of η, one would still believe that that one case is in error. In fact, the precise way in which the various authors had arrived at their choices of the moduli of π was never discussed in Ref. 7, nor in many practical cases need it really be. The calculation that was in "error" was one for which the estimate of the phase shift (modulo π) decreased as one included an additional state, the decrease being by one unit in the third significant figure. It is of course possible that there was an increase of η by just under π, but if only on *a priori* grounds it seems very much more likely that the calculations in question were only reliable to a few units in three significant figures. It is in fact clear from the above discussion that one should rather generally be able to estimate the number of significant figures of the numerical results from the knowledge that the estimate of η must increase as states are added. (It need scarcely be observed, incidentally, that the authors involved were not really concerned with the third significant figure.)

In our previous formulation we were unable to predict inequalities among the phase shifts in various approximations for e^+H scattering for phase shifts containing contributions from other than s states. We noted above, however, that the inequalities (37), which relate phase shifts which contain such contributions, are valid for energies below the pickup threshold. The possibility of proving these additional inequalities is a consequence of the new method of introducing λ. The previous approach required one to prove that $Q(E-H)Q<0$, for Q the projection operator onto all excited states; this we were able to do only for s states. With the present method of introducing λ we need only prove that $Q(E-H_T-T)Q<0$, and this is clearly the case. The additional inequalities that we are now able to prove therefore include $\eta(1s+2s+2p)>\eta(1s+2s)$ and $\eta(1s+2s+2p)>\eta(1s)$ for e^+H scattering at energies below the pickup threshold. The phase shifts necessary to check the above two inequalities are listed in Table 3 of Burke and Smith,[12] for six different energies, and 6×2 inequality predictions are all verified; since the differences between the various phase shifts are relatively small, there is very little possibility that there have been any jumps of π, so that the verification is meaningful. It is perhaps interesting that at one of the energies above the pickup threshold, an energy domain for which the above discussion is not applicable, the phase-shift inequalities are *not* satisfied. (Above the pickup threshold there are of course eigenphase shifts, and not just one phase shift, but the calculation was performed as if one still had a single-channel scattering process.)

We return now to the multichannel problem. One obtains a variety of bounds on combinations of elements of $\mathbf{K}_\theta$ by making different choices for the a_i in Eq. (30). We consider two types of choices, those which isolate a diagonal element and those which lead to an eigenmode.

Setting $\theta=0$ for simplicity, the first choice is simply $a_j=\delta_{ij}$, in which case Eq. (30) becomes

$$dK_{ii}(\lambda)/d\lambda\geq 0. \tag{38}$$

$K_{ii}(\lambda)$ may possibly go through infinity one or more times, that is, $K_{ii}(\lambda)$ may have a number of branches similar, for example, to the tan function, and the monotonicity theorem will be directly useful to us only if we keep track of which branch we are on. One way of doing so, though by no means the only way, is simply to define $\rho_i(\lambda)$ by

$$\tan\rho_i(\lambda)\equiv K_{ii}(\lambda), \tag{39}$$

with multiples of π for $\rho_i(0)$ arbitrarily chosen, and with the understanding that $\rho_i(\lambda)$ is continuous in λ as $K_{ii}(\lambda)$ goes through ∞. We conclude finally that

$$\rho_i{}^P\leq\rho_i{}^{P\star}\leq\rho_i, \tag{40}$$

where, as always, $P^\star$ contains P.

The second choice is the choice $\mathbf{a}(\lambda)=\mathbf{a}^{(j)}(\lambda)$, where $\mathbf{a}^{(j)}(\lambda)$ is the jth (normalized) eigenvector of $\mathbf{K}(\lambda)$, with eigenvalue $\tan\eta^{(j)}(\lambda)$, where $\eta^{(j)}(\lambda)$ is the jth eigenphase shift. Equation (30) then reduces to

$$(d/d\lambda)\tan\eta^{(j)}(\lambda)\geq 0. \tag{41}$$

If we demand that the eigenphase shift $\eta^{(j)}(\lambda)$ be continuous in λ, it follows that[17]

$$\eta^{(j)P}\leq\eta^{(j)P\star}\leq\eta^{(j)},\quad 1\leq j\leq N. \tag{42}$$

4. DISCUSSION

We have seen that the assumption that η is continuous in λ as we go continuously from P space to $P+Q$ space leads to some interesting consequences, but it leaves much to be desired. As already noted, a calculation of the wave function for the given energy and angular momentum and for the actual strength of the potential then determines only η modulo π. Furthermore, since we do not then have an absolute definition of η, there is no place for a theorem such as that proved in Refs. 2 and 11; it was there shown, using the nodal definition, that as a direct consequence of the Pauli principle η for the (spatially antisymmetric) triplet zero-energy scattering of electrons by hydrogen atoms has to be at least π. One can of course introduce an absolute definition of η^P in terms of the nodes of $u_0{}^P$, and then take $\eta(\lambda)$ to be continuous in λ as one expands the space to $P+Q$ space. One would then retain the result that $\eta\geq\pi$, since the Pauli principle generates at least one node in $u_0{}^P$ so that $\eta^P\geq\pi$, and we have $\eta\geq\eta^P$. (On the other hand, it is disturbing that one cannot prove the comparable result for *n-d* scattering.[3]) Furthermore, such a definition might well be able to provide a proof of the surmise of various authors and of Swan[18] in particular concerning the absolute phase shift for the scattering of electrons by atoms with closed shells. The definition is not a particularly natural one however, and one strongly suspects that there must be some more useful and natural definition of phase shifts and, of course, of eigenphase shifts.

APPENDIX

In the present paper we proved that $d\mathbf{K}_\theta(\lambda)/d\lambda$, where it exists, is positive definite for all energies up to the threshold of excitation. (At this threshold the dimensionality of $\mathbf{K}_\theta$ suddenly increases.) On the other hand, a direct generalization to multichannel scattering of the formulation of our previous paper,[7] denoted here by the use of primes, only allows the statement that $d\mathbf{K}_\theta'(\lambda)d\lambda$, where it exists, is positive definite up to the energy $\mathcal{E}_1{}^Q$. The difference in the two results originates in the difference in the way in which λ is introduced. Our previous formulation corresponds to the choice of an optical-model potential $\mathcal{V}'(\mathbf{q},\lambda)$ which differs from $\mathcal{V}(\mathbf{q},\lambda)$ in that there is no λ in the denominator in Eq. (24). It follows that

$$\frac{d\mathcal{V}'(\mathbf{q},\lambda)}{d\lambda}=\int d\mathbf{r}\psi_T(\mathbf{r})\left[VQ\frac{1}{Q(E-H)Q}QV\right]\psi_T{}^\dagger(\mathbf{r}). \tag{A1}$$

As opposed to the right hand side of Eq. (24), the right-hand side of Eq. (A1) is an operator with an obvious definiteness (it is negative definite) only for $E<\mathcal{E}_1{}^Q$, since for $E>\mathcal{E}_1{}^Q$, QHQ has eigenvalues above and below $\mathcal{E}_1{}^Q$. The reactance matrices $K_\theta(\lambda)$ and $K_\theta'(\lambda)$ are in general different from one another, but they agree at the physically significant values of λ, $\lambda=0$ and $\lambda=1$, and the new (unprimed) formulation is clearly more useful since the energy domain of validity is greater.

It is worth noting that $\mathcal{V}(\mathbf{q},\lambda)$ as given by Eq. (24) can obviously be rewritten in a form in which λ and Q appear only in the combination λQ. As λ varies between 0 and 1, we can then think of having turned on Q space continuously.

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[17] Equation (31) represents a monotonicity theorem in $\mathbf{K}_\theta(\lambda)$ and is therefore a generalization of the eigenphase shift monotonicity theorem of R. Bartram and L. Spruch, J. Math. Phys. **3**, 287 (1962). They showed that if $\mathcal{V}_a(q)-\mathcal{V}_b(q)$ is a negative definite operator for all q, where $\mathcal{V}_a$ and $\mathcal{V}_b$ are matrix potentials, with ordered eigenphase shifts $\eta^{(j)}{}_a$ and $\eta^{(j)}{}_b$, respectively, then $\eta^{(j)}{}_a>\eta^{(j)}{}_b$. The significant feature of the present approach is of course that one can prove that $d\mathcal{V}(\mathbf{q},\lambda)/d\lambda$ is negative definite.

[18] P. Swan, Proc. Roy. Soc. (London) **A228**, 10 (1955).