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On the Relation Between Scattering Phase and Bound States*)

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Abstract. The relation between phase shifts and bound states proved by LEVINSON for spherical symmetric potential functions satisfying certain regularity conditions is generalized for arbitrary interactions. The regularity condition of Levinson is replaced by a condition for the behavior of the scattering state wave functions at infinite energy. The proof of the relation given here shows that it is a simple consequence of the orthogonality and completeness relation for the eigenfunctions of the total energy operator.

1. Introduction.

It was shown by LEVINSON[1]) that the scattering phase $\delta(k)$ for S-states in a spherically symmetrical potential $V(r)$ is connected to the number n of bound S-states by the relation

$$\delta(0) - \delta(\infty) = n\pi \tag{1.1}$$

provided the potential satisfies the conditions

$$\left.\begin{aligned} \int_0^\infty r\,|V(r)|\,dr &< \infty \\ \int r^2 |V(r)|\,dr &< \infty \end{aligned}\right\} \tag{1.2}$$

For many applications it would be desirable to have a generalization of this theorem for cases in which the interaction V is not necessarily a diagonal operator in configuration space. For such cases (1·2) will have to be replaced by another condition. It is the purpose of this note to supply such a condition which takes the place of (1.2) and to show that theorem (1.1) still holds under the new restriction imposed on the interaction operator.

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The method of proof will be more elementary than the function theoretical method used by Levinson and others in connection with problems of this kind. In fact in the approach used here we shall show that the relation (1.1) is a simple consequence of the orthogonality and completeness relation for the set of eigenfunctions of the total energy operator $H = H_0 + V$. This is a property which must be assumed to hold for any reasonable quantum mechanical system. It leads us to believe that a theorem analogous to (1.1) must hold even in the case of field theoretical interactions. However, in this case the situation is complicated by the fact that inelastic scattering processes can occur which are accompanied by the production of new particles. The phase shifts for the elastic scattering furnish then no longer a complete description of scattering but they must be supplemented with additional information concerning the probability for the occurrence of various additional particles in the scattering process. This complication has so far prevented us from formulating a correspondingly simple relation for the interactions in field theory.

We shall find it convenient to use the operator formalism of the scattering theory. The simplicity and elegance of this procedure allows the derivation of the basic relations with great ease. Since this formalism has not been generally in use we shall give a brief review[2]) of the main points in Sections 2 and 3.

In Section 4 we shall derive the relation between the wave operator and the phase shift which furnishes the needed link between the S-operator and the wave-operator. With all these preparations out of the way we give the proof of relation (1.1) in Section 5.

2. The Wave-operator.

In scattering theory one usually assumes that the total energy operator H of the system can be separated into two parts

$$H = H_0 + V \tag{2.1}$$

such that H_0 represents the total kinetic energy of the free particles and V their interaction energy. We shall not be concerned here with the complications which occur in multichannel reaction theory where this separation is not possible and shall assume such a decomposition exists.

We shall further assume that the eigenvalues of H_0 as well as H belong to the same continuum starting with a minimum value $E = 0$.

This can always be achieved by a suitable choice of additive constants in H and H_0. The spectrum or H differs from that of H_0 in that H may have in addition a finite of countably infinite number of *bound states*. In order to avoid certain irrelevant complications we shall consider only the case that all the bound states eigenvalues E_α are below the continuum.

$$E_\alpha < 0 . \tag{2.2}$$

The state vectors ω_q of the free particles are eigenstates of the operator H_0

$$H_0\, \omega_q = E(q)\, \omega_q . \tag{2.3}$$

Here q stands for the eigenvalues of a complete set of commuting observables, all of which commute with H_0. They may be a mixture of discrete and continuous variables. The state vectors ω_q are assumed to be normalized in accordance with

$$(\omega_q, \omega_{q'}) = \delta(q, q') . \tag{2.4}$$

The *scattering states* are represented by state vectors of the form

$$\Omega_q = \omega_q + \chi_q \tag{2.5}$$

where χ_q is the scattered wave, which vanishes for those portions in configuration space corresponding to large separations of the particles. The scattering states are solutions of the stationary state SCHRÖDINGER equation

$$H \Omega_q = E(q)\, \Omega_q . \tag{2.6}$$

The *bound states* E_α satisfy

$$H \Omega_\alpha = E_\alpha \Omega_\alpha . \tag{2.7}$$

They are normalized and orthogonal to the scattering states, because of (2.2)

$$(\Omega_\alpha, \Omega_q) = 0 . \tag{2.8}$$

The "wave-matrix", defined by

$$(q\,|\,\Omega\,|\,q') \equiv (\omega_q, \Omega_{q'}) \tag{2.9}$$

can be looked upon as the matrix representation of the "wave operator" Ω, in the complete orthonormal system of the ω_q.

$$(\omega_q, \Omega\, \omega_{q'}) = (q\,|\,\Omega\,|\,q')\,. \tag{2.10}$$

It is therefore the linear operator which transforms the ω_q into the Ω_q according to

$$\Omega_q = \Omega\, \omega_q\,. \tag{2.11}$$

It is now easily recognized that Eq. (2.6) is the projection of the operator relation

$$H\Omega = \Omega H_0 \tag{2.12}$$

on the state vector ω_q. The relation (2.12) is the basic property of the wave operator. It is important to note that it does not define the operator Ω uniquely. Indeed if X is any operator which commutes with H_0 then

$$\Omega_1 = \Omega X \tag{2.13}$$

is also a solution of (2.12). If the system of state vectors (2.5) represents a complete system of scattering states then the converse is also true. We shall refer to the corresponding wave operators as complete.

If Ω is a complete wave operator which moreover satisfies the orthonormal condition

$$\Omega^* \Omega = I \tag{2.14}$$

then the operators $\Omega\,\Omega^*$ and

$$\Lambda = I - \Omega\,\Omega^* \tag{2.15}$$

are projection operators. If Λ is the zero operator then the system of scattering states is already a complete system and Ω is unitary. We shall refer to Λ as the *unitary deficiency*. In terms of the state vectors E_a it may be written as a sum over all bound states

$$\Lambda = \sum_{\alpha=1}^{n} \Omega_\alpha\, \Omega_\alpha^*\,. \tag{2.16}$$

From the orthogonality relation (2.8) follows that every wave operator satisfies

$$\Lambda\Omega = \Omega^* \Lambda = 0\,. \tag{2.17}$$

If the state vectors Ω_α are normalized according to (2.8) then the trace of $\Omega_a \Omega_a^*$ is

$$Tr(\Omega_\alpha \Omega_\alpha^*) \equiv (\Omega_\alpha, \Omega_\alpha) = 1. \tag{2.18}$$

Hence according to (2.16)

$$Tr\,\Lambda = n \tag{2.19}$$

where n is the total number of bound states. If (2.14) holds we may write this last equation as

$$Tr\,[\Omega^*, \Omega] = n\,. \tag{2.20}$$

In this relation we have succeeded in expressing the total number of bound states entirely in terms of the wave-operator. It is therefore the source of the relation (1.1) which we wish to derive.

This result can be extended if the system has integrals, that is operators which commute with the energy operators. In the most important cases a total angular momentum operator $\boldsymbol{J}$ is an integral. Hence we shall assume that there exists such an operator with the usual commutation rules and such that

$$[H, \boldsymbol{J}] = 0 \text{ and } [H_0, \boldsymbol{J}] = 0\,. \tag{2.21}$$

The operators $\boldsymbol{J}^2$ and J_3 are then commuting and can be simultaneously diagonalized with eigenvalues $j(j+1)$ and m $(-j \leqslant m \leqslant j)$ respectively. The projection operator P_j which projects an arbitrary state vector into the subspace of total angular momentum j commutes then also with H and H_0 and hence with Ω. Thus we define

$$\Omega_j = P_j\,\Omega = \Omega\,P_j$$

which satisfies

$$H\,\Omega_j = \Omega_j\,H_0$$

and

$$Tr\,[\Omega_j^*, \Omega_j] = n_j \tag{2.22}$$

where n_j is the number of all the bound states with total angular momentum j.

Since the sum of all projection operators

$$\sum_j P_j = I$$

is equal to the unit operator, we obtain (2.20) from (2.22) by summing over all values of j.

We shall now also formulate the condition which is needed for the validity of Eq. (1.1). In order to do this, we rewrite the equation

$$[\Omega, \Omega^*] = \Lambda$$

in terms of the scattering wave-operator T defined by

$$T = \Omega - 1$$

$$[T, T^*] = \Lambda \tag{2.24}$$

We take the diagonal matrix element of this equation in an arbitrary representation

$$\int_{q'} \{(q|T|q')(q|T|q')^* - (q'|T|q)^*(q'|T|q)\} = (q|\Lambda|q)\,. \tag{2.25}$$

We have indicated the possibly mixed summation and integration over the intermediate variables q' by a symbolic integration sign. For the variables q we choose now the total energy E and a set of additional variables a to complete the system. The integration which occurs in (2.25) can then be written as the integral over E' of the expression

$$F(EE') \equiv \int_{a'} \{(Ea|T|E'a')(Ea|T|Ea)^* - (E'a'|T|E'a')^*(E'a'|T|Ea)\}.$$

We shall require that the integral

$$\int_{E'>E}^{\infty} F(EE')\, dE' < \infty \tag{2.26}$$

be absolutely and uniformly convergent with respect to the parameter E.

The significance of this requirement is the following. The Eq. (2.25) shows that in general a second integration over the variable q cannot be interchanged with the first integration over q'. If it could, then the antisymmetry of the integral would ensure that

$$\int_q (q|\Lambda|q) \equiv Tr\,\Lambda = n\,,$$

is always zero.

As we shall see below there are two reasons for this non-commutative property, one is a singularity of the integral at $E = E'$, and the other is a possibly too weak convergence of the integral at $E \to \infty$. The first reason is always present and is therefore a characteristic property of the scattering operator. The second reason is considered a more or less unusual behaviour of the wave function for very large values of E. For instance it does not hold for interaction potentials which satisfy Levinson's condition (1.2). The condition (2.26) ensures that the contribution of the region $E \to \infty$ to the integral (2.25) vanishes. This will be shown explicitly below.

3. The Scattering Operator.

For convenience of reference we shall mention here four equivalent definitions of the S-operator.

We define for any complete wave-operator Ω, which is a solution of (2.12), a one-parameter family of operators

$$\Omega(\tau) = e^{iH_0\tau}\, \Omega\, e^{-iH_0\tau} \tag{3.1}$$

then the S-operator is defined by the relation

$$\Omega(+\infty) = S\,\Omega(-\infty)\,. \tag{I}$$

A second definition is obtained in terms of the special operators Ω_+ and Ω_- which represent outgoing and ingoing scattered waves and which are given by the integrals[3])

$$\Omega_+ = \lim_{\varepsilon \to +0} \varepsilon \int_{-\infty}^{0} e^{\varepsilon\tau + iH\tau}\, e^{-iH_0\tau}\, d\tau \tag{3.2$_+$}$$

$$\Omega_- = \lim_{\varepsilon \to +0} \varepsilon \int_{0}^{\infty} e^{-\varepsilon\tau + iH\tau}\, e^{-iH_0\tau}\, d\tau\,. \tag{3.2$_-$}$$

These two operators satisfy the initial and final conditions

$$\mathrm{I} = \Omega_+(-\infty) = \Omega_-(+\infty) \tag{3.3}$$

and the orthonormal conditions

$$\Omega_+^*\, \Omega_+ = \Omega_-^*\, \Omega_- = \mathrm{I}\,. \tag{3.4}$$

According to (I) they define the S-operator by either one of the relations

$$S = \Omega_+(+\infty) \qquad S^{-1} = \Omega_-(-\infty)\,. \tag{3.5}$$

A second definition of S is now given by

$$S = \Omega_-^* \, \Omega_+\,. \tag{II}$$

Two more definitions can be given with the help of the operator

$$V(\tau) = e^{iH_0\tau}\, V e^{-iH_0\tau}$$

$$S = \mathrm{I} - i \int_{-\infty}^{+\infty} V(\tau)\, \Omega_+(\tau)\, d\tau \tag{III}$$

$$S^{-1} = \mathrm{I} + i \int_{-\infty}^{+\infty} V(\tau)\, \Omega_-(\tau)\, d\tau\,. \tag{IV}$$

The unitary property and the equivalence of these definitions can be easily proved[4]). It will be convenient for the following to define an operator

$$G_\pm = V\Omega_\pm\,. \tag{3.6}$$

4. Relation Between the Phase Shift and the Wave Operator.

In this section we shall restrict ourselves to a relativistic scalar particle and an interaction operator which does not permit any inelastic scattering (that is there shall be no creation of new particles in the scattering process). The latter condition is rather essential while the former is not. It would be easy to carry through the steps given below with only slight modifications to include the case of particles with spin. For the sake of clarity we shall refrain from doing so.

Under these assumptions the momentum vector $\boldsymbol{k}$ represents a complete system of eigenvalues. We can use them for labelling the energy values and the matrix elements. Because of the rotational symmetry a more convenient system is the set of three variables k, j, m, where the first refers to $k = \sqrt{k_1^2 + k_2^2 + k_3^2}$ the magnitude of the momentum, and j, and m are the total angular momentum and its projection in a fixed space direction. Because of the first of our simplifying assumptions these three variables suffice for the complete identification of the states but it would be easy to include other internal degrees of freedom in the description, such as spin and isotopic spin.

All the operators which commute with $\boldsymbol{J}$ are diagonal in the indices j and m and depend only on j. Hence we can write for the general matrix element of Ω for instance

$$(k\,j\,m\,|\,\Omega\,|\,k'j'm') = (k\,|\,\Omega_j\,|\,k')\,\delta_{jj'}\,\delta_{mm'} \tag{4.1}$$

and similar expressions for all the other matrices which commute with $\boldsymbol{J}$. In all subsequent discussions we shall refer only to the submatrices such as $(k|\,\Omega_j\,|\,k')$ and omit the index j from all equations. It will be understood that the relations obtained will be valid for all j.

The transformation from the variables k to kjm will involve a Jacobian which we shall keep distinct from the matrix elements. Thus we write for the matrix product of two matrices

$$(k\,|AB|\,k') = \int (k\,|\,A\,|\,k''\,k)\,(k''\,|B|\,k')\,k''^2\,dk''. \tag{4.2}$$

The unit matrix is then represented by

$$(k\,|\,\mathrm{I}\,|\,k') = \frac{1}{kk'}\,\delta(k-k')\,. \tag{4.3}$$

The energy is a function $E(k)$ which in the relativistic case would be given by

$$E(k) = \sqrt{k^2+m^2}\,. \tag{4.4}$$

In any case it will be a monotonically increasing function of k. We shall need the Jacobian for the transformation from k to E which we denote by

$$\Delta = \frac{dE}{dk} > 0\,. \tag{4.5}$$

All operators which commute with H_0 are diagonal in k and k'. For instance for the S-matrix we have

$$(k\,|S|\,k') = \frac{1}{k\,k'}\,\delta(k-k')\,S(k)\,. \tag{4.6}$$

The unitary property implies

$$S(k)\,S^*(k) = 1 \tag{4.7}$$

or

$$S(k) = e^{2i\delta(k)}. \tag{4.8}$$

The real quantity $\delta(k)$ is the *phase shift.*

We shall now relate the phase shift to the wave matrix or rather to the matrix representation of the operators G_+ (Eq. (3.6)). According to definitions III and IV we have

$$(k\,|S^{\pm 1}|\,k') = \frac{1}{kk'}\,\delta(k-k') \pm 2\,\pi\,i\,\delta(E-E')\,(k\,|G_\pm|\,k')\,. \tag{4.9}$$

Since

$$\delta(E-E')\,(k\,|G_\pm|\,k') = \delta\,(k-k')\,\frac{1}{\Delta}\,G_\pm(k)\,. \tag{4.10}$$

We obtain

$$S(k)^{\pm 1} = e^{\pm 2i\,\delta(k)} = 1 \pm \frac{k^2}{\Delta}\,2\,\pi\,i\,G_\pm\,(k)\,. \tag{4.11}$$

It will be convenient in the following to define the new functions

$$g_\pm(k) \equiv \pi\,\frac{k^2}{\Delta}\,G\;\;(k) \tag{4.12}$$

and to express the phase shift in terms of these functions

$$g_\pm(k) = -\,e^{\pm i\delta}\sin\delta\,. \tag{4.13}$$

5. Derivation of Relation (1.1).

We are now prepared for the derivation of Eq. (1.1). We start with Eq. (2.24) for any of the submatrices $(k\mid T_j\mid k')$. (In the following we shall work only with the Ω_+ wave operator and omit the $+$.)

$$\int_0^\infty k''^2\,dk'\,\{(k''\,|T|\,k)\,(k''\,|T|\,k') - (k\,|T|\,k'')\,(k'\,|T|\,k'')^*\} = (k\,|\Lambda|\,k')\,. \tag{5.1}$$

From (2.19) follows then

$$\int_0^\infty k^2\,dk\,(k\,|\Lambda|\,k) = n\,. \tag{5.2}$$

We now express the left-hand side in terms of the phase shift via the expression[2]

$$(k\,|T|\,k') = \frac{(k\,|G|\,k')}{E' - E + i\,\epsilon} = -\,2\,\pi\,i\,\delta_+(E - E')\,(k\,|G|\,k')\,. \qquad (5.3)$$

For the δ_+-function we substitute the expression

$$\delta_+(\omega) = \frac{1}{2}\,\delta(\omega) + \frac{1}{2\,\pi\,i}\,\frac{1}{\omega}\,. \qquad (5.4)$$

In the following all denominators are understood as principal values. We now separate the left-hand side of (5.1) into three parts

$$(k\,|A|\,k') = (k\,|A|\,k') + (k\,|B|\,k') + (k\,|C|\,k')\,. \qquad (5.5)$$

The first part arises from products of two δ-functions when (5.4) is substituted into (5.3). This term has the form

$$(k\,|A|\,k') = 2\,\pi^2\,\frac{k\,k'}{\sqrt{\Delta\,\Delta'}}\,\{[G^*(k)\,(k|G|\,k') + (k'|G|\,k)^*\,G(k)]$$
$$-\,[(k\,|G|\,k')\,G^*(k') + G(k)\,(k'\,|G|\,k)^*]\}\,\delta(k - k') = 0\,. \qquad (5.6)$$

It vanishes because only diagonal terms contribute and they vanish identically.

The second term in (5.5) originates in the mixed products of $\delta(\omega)$ and $1/\omega$ in the products of the δ_+-functions. They have the form

$$(k\,|B|\,k') = \frac{\pi\,i}{E - E'}\,\Big\{\Big[\frac{k^2}{\Delta}\,G(k) - \frac{k'^2}{\Delta'}\,G(k')\Big]\,(k'\,|G|\,k)^*$$
$$+\,\Big[\frac{k'^2}{\Delta'}\,G^*(k') - \frac{k^2}{\Delta}\,G^*(k)\Big]\,(k\,|G|\,k')\Big\}. \qquad (5.7)$$

The contribution of these terms to the trace will be evaluated below.

The third term is

$$(k\,|C|\,k') = \int\limits_0^\infty \frac{k''^2\,d\,k''}{(E'' - E)\,(E'' - E')}\,[(k''\,|G|\,k)^*\,(k''\,|G|\,k'$$
$$-\,(k\,|G|\,k'')\,(k'\,|G|\,k'')^*]\,. \qquad (5.8)$$

The trace of this term vanishes

$$\int\limits_0^\infty k^2 (k\,|C|\,k)\,dk = 0 \qquad (5.9)$$

provided the two integrations over k and k'' are interchangeable because the integrand is antisymmetrical. We shall now show that this interchange is permissible provided condition (2.26) is satisfied. In order to see this we write for the integral in (5.8)

$$\int_{E_0}^{\infty} \frac{dE''}{(E''-E)(E''-E')} F(E''; E, E') = (k \mid C \mid k') \qquad (5.10)$$

thereby defining the function $F(E''; EE')$. The minimum energy is $E_0 = E(0)$. In the trace calculation (5.9) only the diagonal terms are involved, hence we define a function

$$\Phi(E'', E) = F(E''; E, E) = -\Phi(E, E''). \qquad (5.11)$$

We now decompose the denominators in (5.8) according to

$$\frac{1}{(E''-E)(E''-E')} = \frac{1}{E-E'} \left(\frac{1}{E''-E} - \frac{1}{E''-E'}\right) \qquad (5.12)$$

and develop the expression

$$\psi(E, E') \equiv \int F(E''; E, E') \left(\frac{1}{E''-E} - \frac{1}{E''-E'}\right) dE'' \qquad (5.13)$$

in powers of $(E - E')$. Only the first order term

$$\psi(E, E') = -(E - E') \int \frac{\Phi(E'', E)}{(E''-E)^2} dE'' + \cdots$$

needs to be considered in view of Eq. (5.9). Using this expression we now obtain for the left-hand side of (5.9)

$$\int_0^{\infty} k^2 (k \mid C \mid k)\, dk = -\int_{E_0}^{\infty} dE \int_{E_0}^{\infty} \frac{\Phi(E', E)}{(E'-E)^2} dE' \qquad (5.10)$$

with

$$\Phi(E', E) = -\Phi(E, E').$$

The explicit expression for $\Phi(E'E)$ is

$$\Phi(E', E) = E' E\, k' k \left\{ |(k' \mid G \mid k)|^2 - |(k \mid G \mid k)|^2 \right\}. \qquad (5.11)$$

On account of the antisymmetry of $\Phi(E'E)$ the expression (5.10) vanishes provided the two integrations can be interchanged. This is the case if the inner integral is uniformly and absolutely convergent. In view of (5.3) this is equivalent to the uniform and absolute convergence of (2.26) which we have explicitly assumed. Hence (5.9) is established.

We now turn our attention to the expression (5.7) which may be expressed in terms of the function

$$g(k) = \frac{k^2}{\Delta} G(k) \tag{5.10}$$

$$(k|B|k') = \frac{i}{E-E'} \{[g(k) - g(k')](k'|G|k)^* + [g^*(k') - g^*(k)](k|G|k')^*\}. \tag{5.11}$$

In the limit $k' \to k$ we have

$$\lim_{k' \to k} \frac{1}{E-E'} [g(k) - g(k')] = \frac{1}{\Delta} g'(k). \tag{5.12}$$

In view of (5.2) and (5.10) we obtain finally

$$n = \frac{i}{\pi} \int_0^\infty \left(g'(k)\, g^*(k) - g(k)\, g'^*(k)\right) dk. \tag{5.13}$$

By expressing this in terms of the phase shift $\delta(k)$ and $\delta'(k) \equiv d\delta/dk$ with (4.13) we find

$$n = -\frac{2}{\pi} \int_0^\infty \delta' \sin^2 \delta\, dk. \tag{5.14}$$

This integral can be evaluated explicitly since

$$\delta' \sin^2 \delta = \frac{1}{2} \frac{d}{dk} \sigma$$

where $\sigma = \delta - 1/2 \sin 2\delta$. We obtain finally

$$n = \frac{1}{\pi} \left(\sigma(0) - \sigma(\infty)\right). \tag{5.15}$$

This relation is equivalent to the relation (1.1) which we wished to prove. In order to show this we put

$$\delta(0) = \alpha$$

$$\delta(\infty) = -n\pi + \alpha', \quad \alpha - \alpha' = \varphi$$

and obtain

$$n = \frac{1}{\pi} (n\pi + \varphi - \sin\varphi)$$

or

$$\varphi = \sin\varphi.$$

The only solution of the last equation is $\varphi = 0$. Thus (1.1) is established.

References.

1) N. Levinson, Kgl. Danske Vid. Selskab, Mat.-Fys. Medd. **25,** N⁰ 9 (1949).

2) For greater details we refer to Chapter 7 of J. M. Jauch and F. Rohrlich, Theory of Photons and Electrons, Addison-Wesley, Cambridge, 1955.

3) The existence of these limits poses a difficult mathematical problem. It has not been possible to formulate the exact conditions which the two operators H and H_0 must satisfy in order to ensure the existence of these limits. If these limits do exist then the S-operator is definable by II for instance and always exists. Hence the solution of this problem would be of considerable importance for the proof of the existence of an S-operator.

4) For details we refer to Chapter 7 of Reference 2, where the equivalence of (I) and (II) and the unitary property are proved. The equivalence of (III) and (IV) with the others can easily be supplied using the fundamental integral identity given in that reference.