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ON THE STRUCTURE OF THE S MATRIX IN THE THEORY OF ELASTIC AND INELASTIC SCATTERING OF NONRELATIVISTIC PARTICLES

Yu. V. TSEKHMISTRENKO

Institute of Physics, Academy of Sciences, Ukrainian S.S.R.

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Integral relations for the components of the S matrix describing a nuclear reaction with two channels (one channel is the elastic scattering of a nonrelativistic particle and the other is inelastic scattering with excitation of the nucleus) are derived from general principles of causality, unitarity, and symmetry, and the analytic properties of some components of the S matrix are established. For simplicity the treatment is confined to the case of spherically symmetrical scattering. In agreement with the results of Wigner[1] and of Baz',[2] the excitation function of the elastic scattering has a break at the threshold of the inelastic process. The form of the excitation function of the inelastic process near threshold is found in the general case.

1. INTRODUCTION

A number of papers[3-6] have been devoted to the determination of the mathematical structure of the S matrix (S function) for the scattering of nonrelativistic particles by a nucleus of finite size or by a potential field. As van Kampen has shown,[4] the S function for the scattering of a nonrelativistic particle by a nucleus of finite size has the form

$$S(\lambda) = e^{-2i\alpha\lambda} \prod_n \frac{1-\lambda/\Lambda_n}{1-\lambda/\Lambda_n^*} \frac{1+\lambda/\Lambda_n^*}{1+\lambda/\Lambda_n} \prod_m \frac{1-\lambda/iP_m}{1+\lambda/iP_m}. \quad (1)$$

The singularities of $S(\lambda)$ in the upper half-plane are simple poles located on the imaginary axis. It is evidently impossible to establish the character of the distribution of poles in the lower half-plane from general considerations. It is also necessary to note that the general requirements of causality, unitarity, and symmetry do not provide the possibility of determining even the order of the poles in the lower half-plane. Generally speaking, despite a widespread impression (cf., e.g., reference 6), there is no basis for believing that they are only simple poles.

It must be remarked that the theory of the elastic scattering of a particle by a nucleus of finite size that has no internal degrees of freedom does not have any concrete applications in atomic and nuclear physics. In actual fact, when the energy of the incident particle is large enough there must necessarily occur a change of state of the bombarded system. Therefore the formula (1) for the S function of the elastic scattering of a particle by a nucleus must be regarded as only an approximate formula that holds for $\epsilon/E \gg 1$, where $E = k^2/2M$ is the energy of the particle and ϵ is the excitation energy of the nucleus. The Breit-Wigner formula, which can be obtained from Eq. (1) (cf. reference 6), is also approximate. Attempted modifications of the Breit-Wigner formula to take into account the channels of reactions other than elastic scattering are much inferior in rigor to the S function of the theory of "pure" scattering. This theory allows us to establish the structure (1) of the S function on the basis of three fundamental principles — causality, unitarity, and symmetry. The formulation of the principles of unitarity and symmetry is quite unambiguous. The causality principle is another matter. After the discussion of this question in the literature we can now regard as established two noncontradictory formulations of the principle of causality: a) the direct formulation proposed by van Kampen[4] (the probability of finding the particle outside the nucleus at the time $t = t_1$ is smaller than this same probability at $t = -\infty$); b) the "indirect" formulation proposed by Heisenberg[7] (the completeness relation must be fulfilled for the wave functions of particles outside the nucleus).

It is a matter of definite interest to establish with mathematical rigor, on the basis of the principles just mentioned, the integral relations between the components of the S matrix (when inelastic-scattering channels are present), and to determine the structure of the components that correspond to the elastic scattering, thus generalizing Eq. (1). In carrying out this program we shall rely on the second formulation of the causality principle. This choice is made on the following considerations: simplicity of the formulation; automatic establishment of the connection of the poles and residues of the S matrix with the eigenvalues of the energy of the system and the normalization coefficients of the bound states; the possibility of a much easier approach to long-range potentials than in the van Kampen formalism. If, unlike Ning Hu,[3] we use exact expressions for the wave functions outside the nucleus in deriving the structure of the S function in the case of a long-range potential, the form of the S function is basically unchanged, except that now not all of its poles will be connected with energy levels of the system (on this point see references 4, 8, and 9).

2. NOTATION. FORMULATION OF SYMMETRY AND UNITARITY PROPERTIES

Let us consider reactions of the type $n + C = n' + C'$, where C is the bombarded system and n and n′ are the incident and scattered particles. For simplicity we shall regard the nucleus C as infinitely heavy. We assume that the energy spectrum of C is purely discrete with nondegenerate levels. We write for the corresponding eigenfunctions $\psi_j(\xi)$, where j numbers off the levels in order of increasing energy and ξ is the internal coordinates of the system C. We take the entire interaction of C with the particle to be spherically symmetrical and localized inside a sphere of radius a. For $r > a$ we can expand the wave function $\Psi_l(E, r, \xi)$ of the system in a series of the functions $\psi_j(\xi)$:

$$\Psi_l(E, r, \xi) = \sum_j \Phi_{lj}(E, r)\psi_j(\xi). \quad (2)$$

As is the usual practice,[10] we call j the channel number and l the number of the open channel. Thus $\Phi_{jj}(E, r)$ contains both the incident and scattered waves, and $\Phi_{l\neq j}(E, r)$ only the diverging wave. Obviously $\Psi_l(E, r, \xi)$ are essentially the same as the functions $\Psi^{(+)}$ introduced by Schwinger and Lippmann.[11] In order hereafter not to obscure the general picture by cumbersome calculations, we shall confine ourselves to the case of just two levels, and let the distance between them be $\epsilon = k_0^2/2M$.

Setting $K = (k^2 - k_0^2)^{1/2}$, we can write more detailed expressions for $\Phi_{lj}(E, r)$:

$$\Phi_{11} = A(e^{-ikr} - S_{11}e^{ikr}), \qquad \Phi_{12} = AS_{12}e^{iKr},$$

$$\Phi_{21} = AS_{21}e^{ikr}, \qquad \Phi_{22} = A(e^{-iKr} - S_{22}e^{iKr}). \quad (3)$$

Obviously we must require that

$$\Phi_{2j} = 0, \quad \text{if } E < \varepsilon. \quad (4)$$

Let us now examine all the conclusions that can be drawn about the properties of the functions S_{lj} without resorting to the completeness relation. We shall regard S_{lj} as a function of k (or K) for positive and negative k (or K). We use the condition of the conservation of the number of particles in the form that expresses the equality of the flux of the converging wave to that of the diverging wave. This leads to the set of relations:

$$|S_{11}|^2 = 1, \qquad (E < \varepsilon), \qquad kK^{-1}|S_{21}|^2 + |S_{22}|^2 = 1,$$

$$|S_{11}|^2 + Kk^{-1}|S_{12}|^2 = 1\,(E > \varepsilon). \quad (5)$$

The next group of relations comes from the obvious fact that under the replacement $k \to -k$ (or $K \to -K$) the function $\Psi_l(E, r, \xi)$ must go over into itself (apart from a constant factor). Here $\psi_j(\xi)$ can of course be regarded as real. These relations are*

$$S_{11}^{-1}(k) = S_{11}(-k), \qquad S_{11}(-k) = -S_{12}(-k)/S_{12}(k),$$

$$S_{22}^{-1}(K) = S_{22}(-K), \qquad S_{22}(-K) = -S_{21}(-K)/S_{21}(K). \quad (6)$$

3. NORMALIZATION AND COMPLETENESS CONDITIONS. INTEGRAL RELATIONS FOR THE COMPONENTS OF THE S MATRIX

The writing of the normalization and completeness relations for $\Psi_l(E, r, \xi)$ is a step beyond the framework of the Schrödinger-equation formalism. Even if we assume that the Schrödinger equation is valid for all r, the completeness relation does not follow from the Hermitian property of the Hamiltonian, as is the case, for example, in the treatment of "pure" elastic scattering.[3] The functions $\Psi_l(E, r, \xi)$ are eigenfunctions of a non-Hermitian operator (cf. e.g., reference 11). This can indeed be seen from the fact that the requirement that there be no converging waves in part of the channels is equivalent to the imposition of a

*If our two states of the target nucleus are due to spin splitting, the relations (6) are changed. In fact it is not difficult to show that with a suitable choice of the quantization axis for the spin the replacement $k \to -k$ (or $K \to -K$) must be accompanied by multiplication of the spin functions ψ_1 and ψ_2 by the matrix σ_2 (in this case ψ_1 and ψ_2 are eigenfunctions of σ_3). As can easily be perceived, this leads to a change of the signs of the fractions in Eq. (6). In the final analysis this difference is unimportant, since these relations are not used in the derivation of the analytical structure of the functions S_{11} and S_{22} that determine all observable quantities.

non-Hermitian boundary condition at infinity. On the other hand, as is well known, the "Hermitian" solution of the Schrödinger equation, which automatically satisfies the completeness condition, cannot describe the scattering problem.

The normalization condition (7) and completeness condition (8) are written down by analogy with the corresponding conditions for "Hermitian" solutions:

$$\int dr \sum_j \Phi_{lj}(E, r)\,\Phi^*_{l'j}(E', r) = \delta(k-k')\,\delta_{ll'}, \qquad (7)$$

$$\int dk \sum_l \Phi_{lj}(E, r)\,\Phi^*_{lj'}(E, r') = \delta(r-r')\,\delta_{jj'}. \qquad (8)$$

From Eq. (7) we can find the coefficient A

$$A = 1/\sqrt{2\pi} \qquad (9)$$

and the relation

$$S_{21}S^*_{11} + kK^{-1}S_{22}S^*_{12} = 0. \qquad (10)$$

For $j = j' = 1$ the condition (8), after some simple manipulations, multiplication by $e^{-ik(r+r')}$, and integration with respect to the variable $\rho = r + r'$ from 2A to infinity ($A > a$), with the use of Eqs. (5) and (6), gives the result (for $E > \epsilon$):

$$|S_{11}|^2 + |S_{21}|^2 = 1, \qquad (11)$$

$$\pi\theta(k)S_{11A}(k) + \pi\theta(-k)S^*_{11A}(-k) + i\int_{-\infty}^{\infty}\frac{S_{11A}(k')}{k'-k}\,dk' + i\int_{k_0}^{\infty} dk'\,\frac{S_{11A}(-k') - S^*_{11A}(k')}{k'+k} = 4\pi i\sum_s \frac{|c_{1s}|^2\exp(2ik_sA)}{k_s-k}, \qquad (12)$$

$$S_{11A}(k) = e^{2ikA}S_{11}(k); \quad \theta(x) = 1 \text{ for } x>0; \quad \theta(x) = 0 \text{ for } x<0. \qquad (13)$$

By analytical calculations one can obtain the integral relation that follows from Eq. (8) for $j = j' = 2$ ($E > \epsilon$):

$$|S_{22}|^2 + |S_{12}|^2 = 2kK^{-1} - 1, \qquad (14)$$

$$\pi\frac{K}{k}S_{22A}(k) - i\int_{k_0}^{\infty}\frac{S^*_{22A}(k')\,dk'}{K+K'} - i\int_{k_0}^{\infty}\frac{S_{22A}(k')\,dk'}{K-K'} + i\int_0^k dk'\,\frac{e^{2iK'A}}{K-K'}|S_{12}(k')|^2 = -4\pi i\sum_s\frac{|c_{2s}|^2\exp(2iK_sA)}{K-K_s}, \qquad (15)$$

$$S_{22A}(k) = e^{2iKA}S_{22}(k). \qquad (16)$$

For $j = 1$, $j' = 2$ the condition (8) gives an extremely complicated integral relation between the components of the S matrix that correspond to different input channels. We shall not concern ourselves with the study of this relation.

Let us turn to the simplification of the relations (12) and (15). From the fact that the relation $|S_{11}|^2 = 1$ becomes invalid for $E = \epsilon$ we can draw the conclusion that S_{11} depends on K. Because the root is multiple valued, S_{11} must be considered on a Riemann surface, which we get by cutting the two k planes from $k = k_0$ to $+\infty$ and from $k = -k_0$ to $-\infty$ and connecting them crosswise along the cuts. Let K take positive values along the upper edges of the cuts in the plane of integration. According to the meaning of the integral $\int_{-\infty}^{\infty}$ in the left member of Eq. (12) the integration is taken along the upper edge of the cut in the right half-plane, and along the lower edge in the left half-plane (the path C, see Fig. 1). Since we intend eventually to apply Cauchy's theorem, we transform our integral in such a way that the integration may also go along the upper edge of the cut in the left half-plane. If we denote the path of integration so obtained by C′, then we have $\int_C = \int_{C'} + \int_{\text{l.c.}}$, where $\int_{\text{l.c.}}$ is the integral around the left-hand cut in the positive direction. We now use the fact that Eq. (12) must be valid for all $A > a$. This means that $\int_{k_0}^{\infty}$ must cancel with $\int_{\text{l.c.}}$. This will happen automatically if

$$S^{(l)}_{11A}(-k) = S^{(u)*}_{11A}(k), \qquad (17)$$

where $S^{(l)}_{11A}(k)$ and $S^{(u)}_{11A}(k)$ are the values that $S_{11A}(k)$ takes on the lower and upper edges of the cuts. Finally the relation (12) takes the form

$$\pi S_{11A}(k) + i\int_{C'}\frac{S_{11}(k')}{k'-k}\,dk' = 4\pi i\sum_s\frac{|c_{1s}|^2\exp(2ik_sA)}{k_s-k}, \qquad (12')$$

where S_{11A} now means only the values of the function on the upper edges of the cuts.

To simplify the relation (15), in the integral $\int_{k_0}^{\infty}$ we must go over to the new variable K. If we write

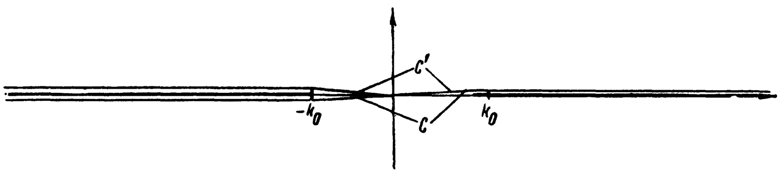

FIG. 1

$$Kk^{-1}S_{22A}(k) = \mathcal{S}_{22A}(K), \tag{18}$$

then Eq. (15) becomes

$$\pi\mathcal{S}_{22A}(K) - i\int_0^\infty \frac{\mathcal{S}^*_{22A}(K')}{K+K'}dK' - i\int_0^\infty \frac{\mathcal{S}_{22A}(K')}{K-K'}dK'$$
$$+ i\int_0^{k_0} \frac{\exp\{2iKA\}}{K-K'}|S_{12}(k)|^2 dk = -4\pi i\sum_s \frac{|c_{2s}|^2\exp\{2iK_sA\}}{K+K_s}. \tag{15'}$$

Let us transform the integral

$$\int_0^\infty dK'\left[\frac{\mathcal{S}^*_{22A}(K')}{K+K'} + \frac{\mathcal{S}_{22A}(K')}{K-K'}\right].$$

We note that $\mathcal{S}_{22A}$ depends also on the function $(K^2 + k_0^2)^{1/2}$. We construct the suitable Riemann surface by cutting the two K planes from ik_0 to $-ik_0$ and joining them crosswise. The plane of integration is characterized by the fact that in it $(K^2 + k_0^2)^{1/2}$ takes positive values on the right-hand edge of the cut. In the integral

$$\int_0^\infty dK' \frac{\mathcal{S}^*_{22A}(K')}{K+K'}$$

we make the change of variable of integration $K' \to -K'$. If we write $\mathcal{S}'_{22A}(K)$ to denote the function $\mathcal{S}_{22A}$ with $(K^2 + k_0^2)^{1/2}$ replaced by $-(K^2 + k_0^2)^{1/2}$, the requirement that A be arbitrary leads to the relation

$$\mathcal{S}^*_{22A}(-K) = \mathcal{S}'_{22A}(K) \tag{19}$$

(otherwise there appears in Eq. (15′) an additional integral from 0 to infinity, which is a function of A and K and must vanish identically, which is impossible).

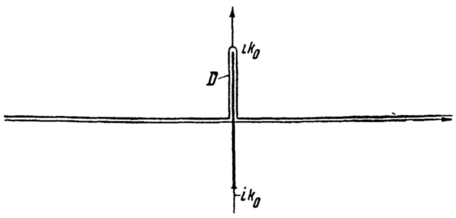

FIG. 2

In the left member of Eq. (15′) let us separate the integral over the path D (see Fig. 2) and some remaining integral over K′ from 0 to ik_0 and over k from 0 to k_0. After a number of transformations it turns out that Eq. (15′) is equivalent to two independent relations:

$$\pi\mathcal{S}_{22A}(K) - i\int_D \frac{\mathcal{S}_{22A}(K')\,dK'}{K-K'} = -4\pi i\sum_s \frac{|c_{2s}'|^2\exp(2iK_sA)}{K-K_s}, \tag{20}$$

$$S_{22}(k) + S_{22}(-k) + |S_{12}|^2 = 0, \quad E < \varepsilon. \tag{21}$$

In Eq. (21) S_{22} and S_{12} are to be understood as the analytic continuations of the corresponding functions into the "nonphysical" region $k < k_0$.

4. CONCLUSIONS ABOUT THE MATHEMATICAL STRUCTURE OF THE S-MATRIX COMPONENTS AND THE BREIT-WIGNER FORMULA

We can now show without difficulty that the functions S_{11A} and $\mathcal{S}_{22A}$ are meromorphic: the former, with respect to k in the part of the k plane above the contour C′ (Fig. 1), and the latter, with respect to K in the part of the K plane above the contour D (Fig. 2). The proof is based on application of Cauchy's theorem and use of the fact that A is arbitrary. Let us consider the integral

$$i\int_{C'} \frac{S_{11A}(k')\,dk'}{k'-k}$$

in Eq. (12′). Adding and subtracting the integral along an infinitely small semicircle passing above the point $k' = k$ and the integral along an arc of infinite radius (to close the path of integration), and using Eq. (12′), we get

$$i\int_{C'} \frac{S_{11A}(k')\,dk'}{k'-k} = -2\pi\sum_s \frac{\operatorname{Res} S_{11A}(k_s)}{k_s-k} - \pi S_{11A}(k)$$
$$-\int_\Gamma \frac{S_{11A}(k')\,dk'}{k'-k}. \tag{22}$$

Thus S_{11A} is a meromorphic function of k in the upper half of the k plane, with simple poles on the imaginary axis, and

$$\int_\Gamma \frac{S_{11A}(k')\,dk'}{k'-k} = 0$$

(Γ is the arc of infinite radius). The analytic continuation of $S_{11A}(k)$ into the lower half-plane can be constructed on the basis of the values of the function on the lower edges of the cuts as defined by Eq. (17). Taking into account Eqs. (5), (6), (13), and (17), we can write the explicit form of $S_{11}(k)$:

$$S_{11}(k) = e^{-2i\alpha_1 k}\frac{f_1(k)K + f_2(k)}{f_1(-k)K + f_2(-k)}\Pi(k) \qquad (0 < \alpha_1 < a), \tag{23}$$

where $\Pi(k)$ is a product of the type of that in Eq. (1), and $f_1(\lambda)$ and $f_2(\lambda)$ are integral functions with no common zeroes, which for real λ have the properties (for all $k > k_0$):

$$\frac{f_1(-k)}{f_2(-k)} = -\frac{f_1^*(k)}{f_2^*(k)}, \qquad \left|\frac{f_1(k)K + f_2(k)}{f_1(-k)K + f_2(-k)}\right|^2 < 1, \tag{24}$$

$$\int_\Gamma e^{i\beta\lambda}\frac{f_1(\lambda)\Lambda + f_2(\lambda)}{f_1(-\lambda)\Lambda + f_2(-\lambda)}d\lambda = \begin{cases}0, & \text{if } \beta > 0\\ \infty, & \text{if } \beta < 0\end{cases}, \tag{25}$$

with β arbitrarily small in absolute value. Obviously only the quantities k_s can be zeroes of $f_1(-\lambda)\Lambda + f_2(-\lambda)$ in the upper half-plane.

In a quite analogous way we can determine the structure of the component $S_{22}(k)$:

$$S_{22}(k) = e^{-2i\alpha_2 K} \frac{g_1(K)\,k + g_2(K)}{g_1(-K)\,k + g_2(-K)} \,\Pi(K) \qquad (0 < \alpha_2 < a). \tag{26}$$

The properties of g are quite analogous to those of f (in the various statements we must make the replacements $f \rightarrow g$, $k \rightleftarrows K$, $\lambda \rightleftarrows \Lambda$).

Let us consider the reaction of the scattering of the particle by the unexcited nucleus ($l = 1$, cf. reference 2). This case is interesting through the presence of the threshold process of the inelastic scattering (with energy loss) of the particle. Using the well known formulas for the integrated effective cross sections for elastic and inelastic scattering (σ_e and σ_r), expressed in terms of S_{11} [see Eq. (23)], we find, in agreement with reference 2, that the excitation function σ_e has a vertical tangent at $k = k_0$ (which corresponds to a break or a point of inflection), and near the threshold σ_r is proportional to $(k^2 - k_0^2)^{1/2}$.

Strictly speaking, of course, these conclusions are valid for not very large energies, when we can neglect the contribution of partial waves with nonzero orbital angular momenta.

SUMMARY

We have succeeded in establishing with mathematical rigor the structure of the S functions of spherically symmetrical elastic scattering of a nonrelativistic particle by a nucleus of finite size when this nucleus has one excited state. In so doing we have used only the physical requirements of conservation of the total number of particles, of symmetry, and of completeness of the system of wave functions outside the nucleus. It has been found that because their arguments are multiple-valued these S functions are not analytic in the whole plane, but S_{11A} is analytic in k above the contour C′ (Fig. 1), and S_{22A} is analytic in K above the contour D (Fig. 2); furthermore in the upper half-plane these functions have simple poles, whose positions are given by the eigenvalues of the energy of the system. From the general form of S_{11} there follow with complete rigor the well known conclusions about the behavior of the excitation functions of elastic and inelastic scattering at the threshold of the inelastic process. The formulas (23) and (26) approximately describe the scattering of slow neutrons by nuclei for which the energy spectrum is characterized by the smallness of the distance between the first two levels in comparison with the distance to the next level. As is well known, such a structure is a property both of many even nuclei and also of many odd nuclei.

In conclusion I express my deep gratitude to Professor A. S. Davydov for a helpful discussion of this work.

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