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On the Connection of the Scattering and Derivative Matrices with Causality*

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The connection between the S matrix and causality suggested by Kronig is analyzed, and it is found that the condition of causality implies that the poles of the analytical functions $S(k)$ are either on the imaginary axis or in the lower half-plane. The possibility of a close connection between the properties of the derivative R matrix and causality is also analyzed. Although all the properties of the R matrix could not be deduced from the requirements of causality, it is considered as an encouraging preliminary result that: (1) The referred distribution of the poles of $S(k)$ can be obtained from the properties of the R matrix. (2) These properties of the corresponding R matrix are unchanged under a transformation $S(k)\to e^{ik\lambda}S(k)$, with λ positive, which preserves the causal nature of the theory.

IT has been suggested recently[1] that the imposition of the causality condition on the scattering matrix (S matrix) formalism[2] for the scattering of particles would result in a supplementary condition for the S matrix. "Causality condition" in this connection means that there can be no scattered wave before the incident wave reaches the scatterer. It seems also natural to surmise that this causality condition is the deeper cause of the properties of the R function[3] (the reciprocal logarithmic derivative of the wave function) found recently by Wigner and Eisenbud.[4] According to the latter, the R matrix is a single-valued analytic function of the energy E. It is real for real E, its poles are all on the real axis and have negative residues. It follows from this condition that, if $R(E)$ is regarded as a function of complex E, its imaginary part has the same sign as the imaginary part of E; we shall call any function with this property an "R function."

We have not succeeded in deriving all the above properties of the R matrix from the requirements of causality. However, we have derived a consequence of these properties, for the S matrix, which may be of considerable interest, since it permits one to understand the behavior of the cross sections within not too wide ranges of the energy.[5] This property is the analog of the one discovered by Foster, Campbell, and Zobel[6] for radio amplifiers and by Krönig and Kramers[7] for the scattering of light on atoms.[8] For these cases the above authors have shown that the poles of the scattering function S are all in the lower half-plane of E.

We shall restrict ourselves in what follows to the S-scattering of nonrelativistic particles by a scatterer of finite radius a, and shall derive first the property in question from the properties of the R function. In the case in question, the connection between the scattering

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[1] R. Kronig, Physica 12, 543 (1946).

[2] J. A. Wheeler, Phys. Rev. 52 (1107(1937); W. Heisenberg, Z. Physik 120, 513, 673 (1943), Z. Naturforsch. 1, 608 (1946).

[3] This surmise made by Professor E. P. Wigner was the starting point of the present investigation.

[4] E. P. Wigner and L. Eisenbud, Phys. Rev. 72, 29 (1947).

[5] P. L. Kapur and R. Peierls, Proc. Roy. Soc. (London) A166, 277 (1938); A. Siegert, Phys. Rev. 56, 750 (1939).

[6] See various articles in Bell System Tech. J., 1922–1924.

[7] H. A. Kramers, Atti. Congr. di Fisica, Como, 1927, p. 545; R. Kronig, Nederland. Tidschr. Naturrk. 9, 402 (1942).

[8] Professor J. A. Wheeler and Mr. J. Toll recently made an extensive analysis of this question and related ones. We are thankful to them for letting us see a preliminary draft of their paper.

function S and the derivative function R is[4]

$$S(k)=e^{-2ika}(1+ikR)/(1-ikR), \tag{1}$$

$$R(k)=\frac{1}{ik}\frac{S(k)e^{2ika}-1}{S(k)e^{2ika}+1}, \tag{1a}$$

where k is the wave number of the incident particle and a is the point at which the reciprocal logarithmic derivative is taken. It follows from (1) immediately that

$$S(-k)=1/S(k) \tag{2}$$

and from the real nature of R, i.e., from $R(k^*)=R(k)^*$ that

$$S(k^*)=1/S(k)^*. \tag{2a}$$

Both these equations are well known and have general validity; they can be derived also directly from the properties of the S function. Equation (2a) corresponds to the unitarity condition for real k.

It follows from (1) that S can have poles only where $1-ikR=0$. Let us write $k=k_1+ik_2$ and $R=R_1+iR_2$; the sign of R_2 is then the same as that of the imaginary part of E, i.e., that of k_1k_2. From $1-ikR=0$ we then obtain the following two equations:

$$1+R_1k_2+R_2k_1=0, \tag{3}$$

$$k_1R_1-k_2R_2=0, \tag{3a}$$

Elimination of R_1 gives

$$k_1+R_2(k_1^2+k_2^2)=0. \tag{3b}$$

It follows that k_1 and R_2 have opposite signs at the poles of S. Since the sign of R_2 is the same as that of k_1k_2, it also follows that S can have poles only where either $k_1=0$ or $k_2<0$.

It is this consequence from (1) and the properties of the R matrix which we shall now derive from the requirements of causality.

For this purpose we form a wave packet of incident S-waves

$$\psi_i(r,t)=\varphi_i(r,t)/r, \tag{4}$$

where

$$\varphi_i(r,t)=\int_0^\infty f(k)e^{-i(Et+kr)}dk. \tag{5}$$

The corresponding scattered wave is

$$\varphi_s(r,t)=\int_0^\infty [S(k)-1]f(k)e^{-i(Et-kr)}dk, \tag{5a}$$

these formulas being valid for $r\geq a$, and $S(k)$ being the S matrix (here an ordinary function). We use natural units: $c=\hbar=1$. We then postulate that if φ_i vanishes at the boundary of the scatterer ($r=a$) for all times $t<t_0$, the same shall hold also for φ_s at all points outside the scatterer. This is equivalent, in view of the continuity equation, to the condition that there will be no scattering before the incident wave reaches the scatterer.

It is convenient to express first the integrals in (5) and (5a) in terms of the energy:

$$\varphi_i(r,t)=\int_0^\infty g(E)e^{-i(Et+kr)}dE, \tag{6}$$

$$\varphi_s(r,t)=\int_0^\infty [S(k)-1]g(E)e^{-i(Et-kr)}dE, \tag{6a}$$

where $g(E)=f(k)M/k$, M being the mass of the particle.

It should be observed here that since in general $S(k)\neq S(-k)$, the analytical continuation of the function $S(E)$ is a two-valued function. As a result, we have to make use of two riemannian sheets in the energy plane. We make the cut along the positive real axis and proceed in the continuation in such a way that the upper and lower half-planes in the first sheet correspond, respectively, to the first and second quadrants of the k plane, and those of the second sheet correspond to the third and fourth quadrants.

We consider then the function $S(E)$ in the first sheet and define the quantity

$$\sigma(\tau,\rho)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}[S(E')-1]e^{-i(E'\tau-k'\rho)}dE', \tag{7}$$

where $\rho\geq 2a$. If there is any pole on the negative real axis (poles on the positive axis are excluded by the unitarity of the $S(k)$ matrix for real k), the expression (7) is to be understood as the limit of the corresponding integral taken along a line in the upper half-plane when this line approaches the real axis. Here we should be careful and analyze the behavior of the integrand of the expression (7), since it is known that the function $S(E)$ has in general a singularity of the type e^{-2ika}/E at the point $-\infty$ of the real E axis, which might "blow out" the integral. The presence of the factor $e^{ik\rho}$ with $\rho\geqslant 2a$ is, however, enough to remove that singularity.

It is clear then that the scattered wave given by expression (6a) can be expressed as

$$\varphi_s(r,t)=\int_{-\infty}^{+\infty}\sigma(t-t';r+r')\varphi_i(r',t')dt' \tag{8}$$

for $r, r'\geqslant a$. In particular for $r'=a$ we have

$$\varphi_s(r,t)=\int_{-\infty}^{+\infty}\sigma(t-t';a+r)\varphi_i(a,t')dt'. \tag{9}$$

Equation (9) expresses the fact that if φ_i is known at all times at the surface of the scatterer, then the scattered wave φ_s is determined for all times at any point outside the scatterer.

It is clear that the causality condition referred to before implies that

$$\varphi_s(r,t)=0 \text{ for } r\geqslant a \text{ and } t<0 \tag{10}$$

if we have

$$\varphi_i(a, t)=0 \text{ for } t<0. \quad (11)$$

As Eq. (10) should hold true regardless of the type of time dependence of the incident wave φ_i for times larger than zero, it follows from Eq. (9) that

$$\sigma(\tau, r+a)=0 \text{ for } \tau<0,\ r\geqslant a \quad (12)$$

or, on account of the definition (7):

$$\int_{-\infty}^{+\infty}[S(E)-1]e^{-i[E\tau-k(a+r)]}dE=0 \quad (13)$$

for all $\tau<0$ and $r\geqslant a$. It is clear that, since $S(E)e^{ik(r+a)}$ is regular at infinity in the upper half-plane of the first sheet, we can close the path of integration on (13) by the upper half-circle at infinity, as both $e^{-iE\tau}$, for $\tau<0$, and $e^{ik(r+a)}$ (a and r are positive) are regular in this half-circle. Since (13) is to be satisfied for any negative τ and for $r\geqslant a$, we see that the analytical function $S(E)$ should have no poles in the upper half-plane of the first riemannian sheet (except the negative real axis). Translating this from the E to the k plane, we see that the causality condition requires that $S(k)$ have no pole in the first quadrant, the positive imaginary axis excluded. This condition on the S matrix is both necessary and sufficient in order to assure the causality.

From here on we continue the analysis by means of the k plane [i.e., use $S(k)$], since the fact that $S(E)$ is two-valued makes the analysis in the E plane more cumbersome.

If we take into account the fact that $S(k)$ satisfies the relation (2b), we find that $S(k)$ will have no poles in the second quadrant either. We have thus obtained from the causality condition the same result which was obtained before from the properties of the R matrix: that the poles of $S(k)$ are either on the imaginary axis or in the lower half-plane.

Although the results of the above analysis seem to indicate that there is a connection between causality and the properties of the R matrix, we were not able to derive all the properties of the R matrix from the causality requirements alone. We think, however, that the following example seems to be an even stronger indication of a deeper connection between causality and the properties of the function R (say, that of being an "R function") and may be of some help for the understanding of this relationship.

Let us call a function $S(k)$ "causal" if from the vanishing of $\varphi_i(r, t)$ of (5) for $t<t_0$, $r=a$, the vanishing of $\varphi_s(r, t)$ for $t<t_0$, $r\geqslant a$ follows. Thus we have shown that the necessary and sufficient condition for the S matrix to be causal is that $S(k)e^{ik\rho}(\rho\geqslant 2a)$ be regular in the upper half of the E-plane (first riemannian sheet).

Now since $e^{ik\lambda}$ for $\lambda>0$ is regular in the upper E-plane, we see that the "causal" nature of $S(k)$ implies the causal nature of the function

$$S_1(k)=S(k)e^{ik\lambda}. \quad (14)$$

Thus it is natural to ask whether the condition that the function $R(k)$ which is related to $S(k)$ by (1a) be an "R function" will entail a similar property for the function $R_1(k)$ which is related to the new "causal" function $S_1(k)$ by

$$R_1=\frac{1}{ik}\frac{S_1e^{2ika}-1}{S_1e^{2ika}+1}. \quad (14a)$$

In other words, we ask whether the transformation (14), which preserves the "causal" nature of the S matrix, does not change the "R function" nature of the corresponding function R. This question will indeed be answered in the affirmative.

Let us first express R_1 in terms of R:

$$R_1(k)=\frac{k^{-1}\tan(k\lambda)+R(k)}{1-k\tan(k\lambda)R(k)}. \quad (15)$$

Now we observe that the homographic transformation,

$$W=\frac{k^{-1}\tan(k\lambda)+Z}{1-k\tan(k\lambda)Z},\quad \lambda>0, \quad (16)$$

is such that:

(a) If the imaginary part of k^2 (or of R) is positive, any number Z with positive imaginary part goes into a number W with positive imaginary part.

(b) If the imaginary part of k^2 is negative, any number Z with negative imaginary part goes into a W with negative imaginary part.

This proves that, if R is an "R function," then R_1 given by (15) is also an "R function."

We understand that Professor John A. Wheeler has found, using a somewhat different approach, some of the results given in this paper.

We wish to express our thanks to Professors E. P. Wigner and V. Bargmann for many helpful discussions.