DERIVATIVE MATRIX AND SCATTERING MATRIX

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I.- INTRODUCTION

R. Kronig[1] was the first to point out, on the basis of his and Kramers' work[2], that the principle of causality must entail some properties of the collision and scattering matrices. Starting from Kronig's suggestion, Schutzer and Tiomno[3] gave, for non relativistic particles, a derivation of the well known theorem[4] that the poles of the scattering function $S(k)$ lie either in the lower half plane or on the imaginary axis of k. Schutzer and Tiomno's work has been extended, since, by Toll and by Van Kampen[5] to the case of relativistic particles with zero rest mass which formed also the subject of Kronig's and Kramer' early considerations[2]. Results similar to these were obtained in the course of the last years also in communication engineering, following the pioneering work of Campbell, Zobel and Foster[6], and of Cauer[7],

by Brune[8], by Fränz[9] and, particularly, by Richards[10]. It was possible to derive from the principle of causality also that $S(k)$ satisfies the further well known equations[4]

$$S(k)\ S(-k) = 1 \qquad S(k)\ (S(k^*))^* = 1 \qquad (1)$$

and that if ρ is larger than the range a_{min} of the scattering forces

$$S(k)\ e^{2ik\rho} < \infty \qquad (\text{for } \rho > a_{min},\ \mathrm{Im}k > 0) \qquad (2)$$

is uniformly bounded in the upper half plane of k.

The above theorems about the function $S(k)$ have been derived by Schutzer and Tiomno also from the properties of the $R(E)$ function. In the case of simple scattering with definite angular momentum, which is the only one with which Schutzer and Tiomno's paper as well as the present one deal, $R(E)$ is the ratio of the wave function to its radial derivative, at a point $r = a > a_{min}$ outside the range of the scattering forces. Hence $R(E)$ depends not only on E but also on a. However, this quantity will be considered to be a constant in all that follows. If the wave function outside a has the form $A \sin kr + B \cos kr$, the connection between R and the scattering function becomes

$$S(k) = e^{-2ika}\ \frac{1 + ik\,R(k^2)}{1 - ik\,R(k^2)} \qquad (3)$$

$R(E)$ as function of $E = k^2$ is a single valued real function[11] of E

$$R(E^*) = (R(E))^* \qquad (4)$$

which has, for finite E, no other singularities but poles[12] and its imaginary part is positive in the upper, negative in

the lower half plane. It follows from this property that the poles of R are all at real E and have negative residues. A function R(E) which has these properties will be called a permissible R. One can then formulate Schutzer and Tiomno's secondary result also by stating that an S(k), derived by (3) from a permissible R, has all the properties given in the first paragraph.

The present note will first inquire whether, conversely, the properties of S(k) enumerated above suffice to establish the properties of R. This can easily be seen as far as the single valued and real nature (4) of R are concerned but will be answered in the negative concerning the theorems about the poles and residues of R. Hence we shall inquire for necessary conditions which S(k) must fulfill in order to be derivable, by (3), from a permissible R. This will lead to an alternation theorem for the poles of S which are on the imaginary axis.

II.- S(k) WHICH DO NOT LEAD TO PERMISSIBLE R(E)

A rather simple general expression which always satisfies the requirements (1) and (2) for scattering functions is

$$S(k) = \frac{f(ik)}{f(-ik)} e^{-2ibk} \qquad (5)$$

in which

$$f(x^*) = f(x)^* \qquad (5a)$$

is a real function, $b < a_{min}$ and

$$\frac{f(-k_1 + ik_2)}{f(k_1 - ik_2)} < \infty \qquad \text{for} \quad k_1 > 0 \qquad (5b)$$

is bounded if $k_1 + ik_2$ is in the right half plane. These conditions are clearly all satisfied if $f(x)$ is a real polynomial of x, i.e., $f(ik)$ a real polynomial of ik. Furthermore, the poles of S will have the proper location if the roots of $f(x)$ are all either real or lie in the left half plane. Scattering functions of this form play an important role in communication engineering[6,7]. Our procedure will be to calculate the R from (5) by means of the inversion of (3)

$$R = \frac{i}{k} \frac{1 - S\, e^{2iak}}{1 + S\, e^{2iak}} \qquad (a > a_{min}) \qquad (6)$$

and ascertain whether the R obtained in this way

$$R = \frac{k^{-1}\ tg\ \alpha k + F(k)}{1 - F(k)\ k\ tg\ \alpha k}\ ; \qquad (7)$$

where

$$\alpha = a - b > 0 \qquad (7a)$$

$$F(k) = \frac{f(ik) - f(-ik)}{ik\ [f(ik) + f(-ik)]} \qquad (7b)$$

give a permissible R function in the sense of the second paragraph of the introduction.

Clearly, $k^{-1}\ tg\ \alpha k$, $k\ tg\ \alpha k$ as well as $F(k)$ are real even functions of k. It follows that the R of (7) is a single valued real function of $k^2 = E$ which can have, furthermore, no essential singularities for finite E. This point was noted already by Schutzer and Tiomno[3]. The only further conditions which remain to be verified concern, therefore, the position of the poles of R and their residues. It easily follows from the general theorems on R functions[11]

that these conditions would also be satisfied if F as well as EF were themselves permissible R functions. This, however, is not the case in general.

In order to find a simple case in which (7) is not permissible we note that this is a continuous function of α at $\alpha = 0$ in every finite region of k except possible where $F(k)$ has a singularity. However, if $F(k)$ should have a negative imaginary part for a k for which k^2 has a positive imaginary part, this will be true also for a sufficiently small finite α and (7) will represent, for such an α, a not permissible R. Hence (7) can represent a permissible R for all permissible S only if this is true also for the expression which one obtains by setting $\alpha = 0$ in (7), i.e. if it is true for the F of (7b). One sees that the permissible nature of F is a necessary condition for the permissible nature of R at all admissible a and b while the permissible nature of F and EF would be a sufficient condition.

The two simplest f which give an S satisfying all conditions but may give a not permissible F and, hence, a not permissible R, are

$$f(-ik) = -k^2 - 2ibk + c \qquad (8a)$$

with either $b > 0$ or $b^2 > c$ and

$$f(-ik) = (-k^2 - 2ib_1k + c_1)(-k^2 - 2ib_2k + c_2) \qquad (8b)$$

in which either $b_1 > 0$ or $b_1^2 > c_1$, and either $b_2 > 0$ or $b_2^2 > c_2$. If the b is positive, the sum of the roots of $f(x) = x^2 + 2bx + c$ is negative and they must lie in the left half plane if they are complex. If $b^2 > c$, both roots are real. The same considerations apply to (8b). It follows that the S obtain from (8a) or (8b) by means of (5) will satisfy

all conditions of the first paragraph. Nevertheless, the

$$F(k) = \frac{2b}{c-k^2} = \frac{2b}{c-E} \qquad (9a)$$

will have a negative residue at its pole $E = c$ only if b is positive. In the other case, in fact, F is "antipermissible", i.e. it has a negative imaginary part in the upper, a positive one in the lower half plane. Similarly, the F obtained from (8b) by means of (7b)

$$F = \frac{-2(b_1 + b_2)\, E + 2b_1c_2 + 2b_2c_1}{E^2 - (c_1 + c_2 + 4b_1b_2)\, E + c_1c_2} \qquad (9b)$$

will have complex poles if $4c_1c_2 > (c_1 + c_2 + 4b_1b_2)^2$ which is not incompatible with the conditions enumerated above. One can put, for instance $c_1 = c_2 = -2$, $b_1 = b_2 = 1$. In this case, the imaginary part of F will assume arbitrarily large positive values at some points of the lower half plane and arbitrarily large negative values at the opposite points of the upper half plane. We can conclude from these examples that (1) and (2), together with the conditions for the location of the poles of S, do not guarantee the permissible nature of the R obtained from the S.

III.- ALTERNATION THEOREM

Since the conditions on S which were enumerated in the first paragraph of the introduction do not necessarily lead to a permissible R, it is natural to ask whether the condition to yield a permissible R leads to simple additional properties of S. This will be found to be the case.

All the poles Z_ν of R are real and the zeros x_ν

also lie on the real axis; there is one zero between any two successive poles[13]. Let Z_0, Z_{-1}, Z_{-2},... be the negative poles in decreasing order, Z_1, Z_2, Z_3,... the positive poles in increasing order, the zero between Z_ν and $Z_{\nu+1}$ shall be denoted by x_ν

$$Z_\nu < x_\nu < Z_{\nu+1} \tag{10}$$

$$Z_0 \leqslant 0 < Z_1 \tag{10a}$$

x_0 can be positive or negative. Then, every permissible R allows a product expansion[14]

$$R(E) = C \frac{E - x_0}{E - Z_0} \Pi \frac{1-E/x_\nu}{1-E/Z_\nu} \Pi \frac{1-E/x_{-\nu}}{1-E/Z_{-\nu}} \tag{11}$$

with positive real C. The two products Π can be finite or infinite.

It follows from (3) that the poles of S satisfy the equation

$$1 - ik\,R(k^2) = 1 + \kappa\,R(-\kappa^2) = 0 \tag{12}$$

where $\kappa = -ik$. With (11), this gives

$$(\kappa^2+Z_0) \Pi (1+\kappa^2/Z_\nu) \Pi (1+\kappa^2/Z_{-\nu}) =$$

$$= -C\kappa(\kappa^2 + x_0) \Pi (1 + \kappa^2/x_\nu) \Pi (1+\kappa^2/x_{-\nu}) . \tag{13}$$

The left side of this equation is shown as function of the real κ, schematically, in the upper part of Figure 1; the right side of (13) in the two lower diagrams. The first product Π is positive in both cases for all real κ. The zeros of the left side lie at $\kappa = \pm\sqrt{(-Z_{-\nu})} = \pm\zeta_\nu$ with $\nu = 0, 1, 2,...$ and the whole left side changes at every ζ_ν and $-\zeta_\nu$; it

is negative at $\kappa = 0$. The zeros of the right side lie at $\kappa = 0$ and $\kappa = \pm\sqrt{(-x_{-\nu})} = \pm\xi_\nu$ with $\nu = 0, 1, 2$ if $x_0 < 0$ and $\nu = 1, 2, 3, \ldots$ if $x_0 > 0$. In the former case the right side is positive between 0 and ξ_0; in the latter case it is negative between 0 and ξ_1.

Let us take up the second case ($x_0 > 0$) first. It follows from (10) that

$$0 < \zeta_0 < \xi_1 < \zeta_1 < \xi_2 < \zeta_2 \quad \ldots \qquad (14)$$

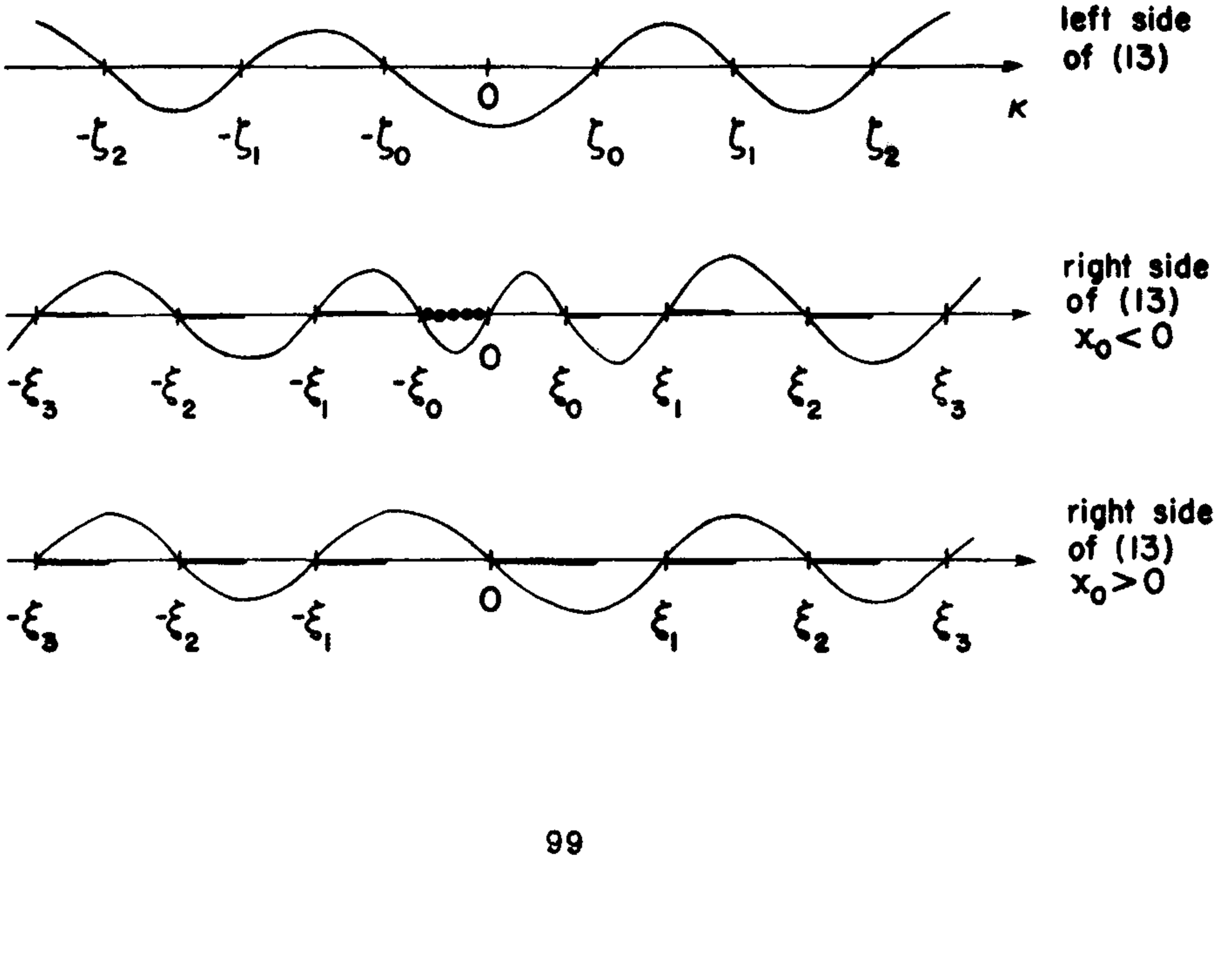
Hence (13) will have a solution κ_0 between 0 and ζ_0 because the left side of (13) increases in this interval from a negative value to zero; the right side drops from zero to a negative value. On the other hand, (13) can have no root between ζ_0 and ξ_1 because the two sides of (13) have opposite signs in this interval. Again, there will be a root $\xi_1 < \kappa_1 < \zeta_1$ and in general in every interval (ξ_ν, ζ_ν). For negative κ, the situation will be opposite: the roots $-\kappa_\nu'$ will be so situated that $\zeta_{\nu-1} < \kappa_\nu' < \xi_\nu$. One can summarize this by stating that the absolute values of the positive imaginary poles $k = i\kappa_0, i\kappa_1', i\kappa_2, \ldots$ alternate with those of the negative imaginary poles $k = -i\kappa_1', -i\kappa_2', -i\kappa_3', \ldots$

$$0 < \kappa_0 < \kappa_1' < \kappa_1 < \kappa_2' < \kappa_2 < \kappa_3' \quad \ldots \qquad (15)$$

The situation is very similar if x_0 is negative, except that, in this case, either (15) holds or there can be two negative imaginary poles $k = -i\kappa_0'$ and $k = -i\kappa_0''$ the absolute values of which are both smaller than that of the smallest positive imaginary pole κ_0.

The situation as described above certainly seems the most natural one and can be expected to be the usual one. It

is conceivable, however, that instead of the a single pole between 0 and ζ_o, for instance, one has three poles or, in fact, any odd number of poles. This can happen if the curves of Figure 1 are not as smooth as drawn but show appreciable curvature. In such a case, every heavily drawn interval in Figure 1 can contain an arbitrary odd number of poles while the $(-\zeta_o, 0)$ interval, i.e. the first negative interval, will contain an even number of poles. The final rule which emerges is therefore as follows. If one orders the purely imaginary poles of S according to their absolute value, one first finds an even number (or zero) of negative imaginary poles, then an odd number of positive imaginary poles, then an odd number of negative imaginary poles, and odd numbers of positive and of negative imaginary poles then continue to alternate.



The above alternating rule is by no means a sufficient condition for S to yield, by (6), a permissible R; it is only a necessary condition. If the properties of S, enumerated in the first paragraph, suffice to ensure the principle of causality[3], this principle cannot suffice to derive the properties of R, given in the second paragraph. Since these properties of R follow from the possibility to define a local probability and flux density, it would be interesting to ascertain whether they remain valid for particles, such as the light quantum, for which no such local densities can be defined.

FOOTNOTES

1. R. Kronig, Physica 12, 543 (1946). This remark gave the original stimulus to the article of reference 3 and hence also to the present paper.
2. H.A. Kramers, Atti Cong. di Fisica Como 1927, p. 545, R. de L. Kronig, Ned. T. Natuurk 9, 402 (1942).
3. W. Schutzer and J. Tiomno. Phys. Rev. 83, 249 (1951).
4. For the older literature cf Chr. Moeller, K. Danske Vidensk.Selsk. 23, No. 1 (1945); 22, No. 19 (1946).
5. Personal communication.
6. G. A. Campbell, Bell System Tech.Journ. 1, No. 2 (1922), O.J. Zobel, ibid 2, 1 (1923), R. M. Foster, ibid 3, 259 (1924).
7. W. Cauer, Arch.Elektrotechnik 17, Chapter II (1926), Sitzungsber.Preuss.Akad. 1927, 1931, Math. Ann. 105, 101 (1931), 106, 369 (1932), Elektrische Nachrichten Technik 9, 157 (1932).
8. O. Brune, Journ. of Math. and Phys. 10, 191 (1931). This article contains numerous errors.

9. K. Franz, Elektrische Nachrichten Technik 21, 8 (1944)

10. P.I. Richards, Duke Math. Journ. 14, 777 (1947)
I am much indebted to Dr. N. Greenspan for the last three references.

11. The properties of R are discussed in some detail in the writer's article, Ann. of Math. 53, 36 (1951) and in a forthcoming article Amer. Math. Monthly. The concept of the derivative matrix (and derivative function) was used by E. P. Wigner and L. Eisenbud, Phys. Rev. 72, 29 (1947).

12. S, as function of E, has a branch point at $E = 0$ but is a single valued function of k in the case of pure scattering and will therefore always be considered to be a function of k. On the other hand, R is a single valued function of both $E = k^2$ and k in the non-relativistic case but its properties are simpler if it is considered to be a function of E and will always be considered to be a function of E. In the relativistic case, or if, in addition to scattering, reactions are also possible, (i.e. if S and R become matrices), S has in general several branch points and R is single valued only as a function of E.

13. Cf. e.g. the first article of reference 11.

14. The product expansion (10) for somewhat specialized R was given in references 9 and 10. A general proof is given in the second reference of 11.