S-Matrix and Causality Condition. I. Maxwell Field

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The general aim is to obtain maximum information about the S-matrix with a minimum of assumptions concerning the interaction. This program is carried through for the scattering of the electromagnetic field by a fixed center. The center is assumed spherically symmetric and of finite size, so that the causality condition can be applied. From this condition it follows rigorously that the S-matrix has a one-valued analytic continuation, whose only singularities are poles in the lower half-plane, and whose behavior at infinity can be specified. Particular consequences are: (i) the analytic properties of Wigner's function R; (ii) the integral relation connecting real and imaginary parts of S; (iii) relations connecting the sum of the oscillator strengths with the scattering cross section.

I. INTRODUCTION

THE S-matrix was introduced by Heisenberg[1] as a device to describe scattering processes without any specific assumptions about the interaction. To compute the S-matrix in a particular case, of course, a certain interaction has to be assumed. But some general properties (e.g., unitarity) could be formulated in terms sufficiently general to raise the hope that they were of more universal character. For their derivation, however, a more or less specific model had to be used.[1,2] This is justifiable from a heuristic point of view, but an attempt to treat the S-matrix without reference to any particular kind of interaction seems none the less desirable. The problem is then no longer: what mathematical properties of S can be derived from the various physical properties of the interaction?—but rather: how are the mathematical properties of S related to actual observations?

Since this question cannot be answered here in its full generality, we shall restrict our investigations in three respects. In the first place, only the scattering of an electromagnetic field by a fixed center is treated. The field is classical, which is equivalent to saying that only the one-photon part is taken into account.[3] Secondly, the scattering center (which for brevity will be called the "core") is assumed to be spherically symmetric, and also invariant with respect to space reflection. In terms of observations, this amounts to assuming that not only multipole waves of different order l, but also the electric and the magnetic multipoles are scattered independently. Thirdly, it is supposed that in all experiments the energy and the frequency (energy per photon) are conserved, and that the "causality condition" is satisfied. These properties are not held to be self-evident, but without these restrictions the analysis would be very cumbersome.

The causality condition states that no scattered wave can be observed until the incident wave packet has reached the core. Obviously it can only be applied when the core has a finite size, which will therefore be postulated throughout this work. This condition turns out to be a powerful aid, because it entails the analytic character of the S-matrix (as a function of the frequency). On the basis of a similar condition, Toll and Wheeler[4] derived the Kramers-Kronig dispersion formula[5,6] for the propagation of light in a medium. It has also been used in electric circuit theory,[7] and its application to the S-matrix was suggested by Kronig.[8]

Schützer and Tiomno[9] considered the scattering of a Schrödinger particle by a core of finite size. In that case, however, the Fourier decomposition of any solution of the Schrödinger equation contains only components with positive E, so that it is impossible to construct a wave packet that is rigorously zero up to a certain time. Hence, the causality condition has to be formulated by means of wave packets that are arbitrarily small in the past, which would make the mathematical treatment more involved. Complications of the same kind arise for relativistic particles, because the values of E between $-m$ and $+m$ are lacking in the Fourier decomposition. This is the reason why we here treat the electromagnetic field only.

Many of the resulting formulas have been found previously starting from more or less special models,[10–12] usually for the scattering of nonrelativistic particles by nuclei. A rather more general approach was attempted by Heisenberg[13] and by Hu,[14] based on the complete-

[1] W. Heisenberg, Z. Physik **120**, 513, 673 (1943).
[2] C. Møller, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **23**, No. 1 (1945); **22**, No. 19 (1946).
[3] H. A. Kramers, "Quantentheorie des Elektrons und der Strahlung," *Hand- und. Jahrbuch der Chem. Physik* (Akademische Verlagsgesellschaft, Leipzig, 1938), p. 439.
[4] J. S. Toll and J. A. Wheeler, unpublished; J. S. Toll, thesis, Princeton, 1952.
[5] H. A. Kramers, Atti cong. intern. fisici, Como, 1927, Vol. 2, p. 545.
[6] R. de L. Kronig, J. Opt. Soc. Am. **12**, 547 (1926).
[7] B. Gross, Phys. Rev. **59**, 748 (1941); R. Kronig, Nederland. Tijdschr. Natuurk. **9**, 402 (1942).
[8] R. Kronig, Physica **12**, 543 (1946).
[9] W. Schützer and J. Tiomno, Phys. Rev. **83**, 249 (1951).
[10] G. Breit and E. Wigner, Phys. Rev. **49**, 519 (1936); P. L. Kapur and R. Peierls, Proc. Roy. Soc. (London) **A166**, 277 (1938); A. J. F. Siegert, Phys. Rev. **56**, 750 (1939); E. P. Wigner and L. Eisenbud, Phys. Rev. **72**, 29 (1947); M. Moshinski, Phys. Rev. **81**, 347 and **84**, 525 (1951); J. Humblet, Mém. Soc. Roy. Scient. Liège **12**, fasc. 4 (1952).
[11] H. A. Bethe and G. Placzek, Phys. Rev. **51**, 450 (1937).
[12] Feshbach, Peaslee, and Weisskopf, Phys. Rev. **71**, 145 (1947).
[13] W. Heisenberg, Z. Naturforsch. **1**, 608 (1946).
[14] N. Hu, Phys. Rev. **74**, 131 (1948).

ness of the solutions of the wave equation (which is related to the causality condition). However, since they used the asymptotic expression instead of the wave function itself, this may lead to incorrect results, as exemplified by the existence of redundant zeros.[15]

II. DEFINITION OF THE S-MATRIX

The S-matrix is defined, in general terms, as the matrix that transforms the wave function describing the ingoing field into the wave function of the outgoing field. For a more specific definition the free-field equations have to be used, and a particular set of field quantities has to be chosen in which to express the transformation. In the present section this is briefly done for the Maxwell field, and the well-known properties (9) of S are derived.

The electromagnetic field outside the scattering center may be described by the complex vector field $\mathbf{F}=\mathbf{E}+i\mathbf{H}$, obeying the equations (we put throughout $c=1$)

$$\partial\mathbf{F}/\partial t=-i\,\mathrm{curl}\mathbf{F},\quad \mathrm{div}\mathbf{F}=0.$$

The solutions are conveniently expressed in terms of a complex Debye potential[16,17] $u(\mathbf{r},t)$:

$$\mathbf{F}(\mathbf{r},t)=(\mathrm{curl}+i\partial_t)\,\mathrm{curl}\,\mathbf{r}u(\mathbf{r},t),\tag{1}$$

$$(\Delta-\partial_t^2)u=0.\tag{2}$$

On introducing polar coordinates $\mathbf{r}=(r,\theta,\phi)=(r,\Omega)$ the asymptotic part of any solution of (2) is a superposition of multipole waves

$$u(r,\Omega,t)\simeq\sum_{l,m}\frac{2Y_{lm}(\Omega)}{[2l(l+1)]^{\frac{1}{2}}}\int_{-\infty}^{+\infty}\left\{B_{lm}(k)\frac{e^{ikr}}{ikr}-(-1)^lA_{lm}(k)\frac{e^{-ikr}}{ikr}\right\}e^{-ikt}dk.\tag{3}$$

The first term consists of outgoing waves, the second of ingoing waves. The sign in front of $A_{lm}(k)$ has been chosen such that absence of scattering is characterized by $A_{lm}(k)=B_{lm}(k)$. The asymptotic expression of the field $\mathbf{F}$ can be derived from (3) by means of (1); one finds $F_r=0$, and

$$\begin{aligned}F_\theta+iF_\varphi&=\frac{4}{r}\sum_{lm}\left(\frac{\partial}{\partial\theta}+\frac{i}{\sin\theta}\frac{\partial}{\partial\varphi}\right)\times\frac{(-1)^lY_{lm}(\Omega)}{[2l(l+1)]^{\frac{1}{2}}}\int_{-\infty}^{+\infty}A_{lm}(k)e^{-ik(r+t)}dk,\\F_\theta-iF_\varphi&=\frac{4}{r}\sum_{lm}\left(\frac{\partial}{\partial\theta}-\frac{i}{\sin\theta}\frac{\partial}{\partial\varphi}\right)\times\frac{Y_{lm}(\Omega)}{[2l(l+1)]^{\frac{1}{2}}}\int_{-\infty}^{+\infty}B_{lm}(k)e^{ik(r-t)}dk.\end{aligned}\tag{4}$$

[15] S. T. Ma, Phys. Rev. **71**, 195 (1947); J. Meixner, Z. Naturforsch. **3a**, 75 (1948).
[16] P. Debye, Ann. Physik **30**, 57 (1909).
[17] J. Meixner, Z. Naturforsch **3a**, 507 (1948).

From this there follows for the total energy entering a sphere with large radius r

$$\int_{-\infty}^{+\infty}dt\oint r^2d\Omega\frac{1}{16\pi}|F_\theta+iF_\varphi|^2=\sum_{lm}\int_{-\infty}^{+\infty}|A_{lm}(k)|^2dk;\tag{5}$$

and a similar expression with $B_{lm}(k)$ for the outgoing energy.

Let it be supposed that these energy amounts are finite. It then follows from the square integrability of $F_\theta+iF_\varphi$ and $F_\theta-iF_\varphi$ that a Fourier expansion (4) is possible. On the other hand, there is no physical justification for imposing square integrability on u; the expansion (3) should therefore be considered as a formal abbreviation for the corresponding expansion (4) of $\mathbf{F}$. Hence we shall only deal with incident wave packets of finite energy; they correspond to square integrable $A_{lm}(k)$. The square integrability of $B_{lm}(k)$ then follows from the conservation of energy.

The coefficients $A_{lm}(k)$ and $B_{lm}(k)$ are connected by a relation expressing the scattering properties of the core. The following properties will be postulated throughout.

(a) *Superposition*

The connection is linear in the following restricted sense: to an ingoing wave $A_{lm}(k)=A_{lm}^{(1)}(k)+A_{lm}^{(2)}(k)$ corresponds the outgoing wave $B_{lm}(k)=B_{lm}^{(1)}(k)+B_{lm}^{(2)}(k)$; and to $cA_{lm}(k)$ corresponds $cB_{lm}(k)$ if c is a *real* constant. From this it follows that

$$B_{lm}(k)=\sum_{l'm'}\int_{-\infty}^{+\infty}\{S'(k;l,m|k';l',m')A_{l'm'}(k')+S''(k;l,m|k';l',m')A_{l'm'}^*(k')\}dk,$$

where S' and S'' are integral kernels that are not more singular than $\delta(k-k')$.

(b) *Spherical Symmetry*

On a rotation about the origin, $A_{lm}(k)$ and $A_{l,-m}^*(k)$ transform like Y_{lm}^*, i.e., diagonal in l and irreducible in m. Hence

$$S'(k;l,m|k';l',m')=\delta_{ll'}\delta_{mm'}S_l'(k|k'),$$
$$S''(k;l,m|k';l',m')=\delta_{ll'}\delta_{m,-m'}S_l''(k|k').$$

(c) *Conservation of Frequency*

The frequency of the outgoing wave is equal to that of the ingoing wave:

$$S_l'(k|k')=\tfrac{1}{2}\delta(k-k')S_l^{(1)}(k)+\tfrac{1}{2}\delta(k+k')S_l^{(2)}(k),$$
$$S_l''(k|k')=\tfrac{1}{2}\delta(k-k')S_l^{(3)}(k)+\tfrac{1}{2}\delta(k+k')S_l^{(4)}(k).$$

(d) *Invariance for Space Reflection*

This implies that if $\mathbf{F}(\mathbf{r},t)$ is a possible scattering state, so is

$$\bar{\mathbf{F}}(\mathbf{r},t)\equiv\mathbf{F}^*(-\mathbf{r},t).$$

By substituting in (4) one finds

$$\bar{A}_{lm}(k)=(-1)^l A_{l,-m}{}^*(-k),\ \bar{B}_{lm}(k)=(-1)^l B_{l,-m}{}^*(-k).$$

In order that $\bar{A}$ and $\bar{B}$ satisfy the same relation as A and B, it is necessary that

$$S_l{}^{(j)}(-k)=S_l{}^{(j)*}(k) \quad \text{for} \quad j=1, 2, 3, 4.$$

The relation between A and B is now determined by four complex functions $S_l{}^{(j)}(k)$ of $k>0$ for each $l\geqslant 1$. For our purpose to find more information about these functions, it is sufficient to consider one particular l and to take $m=0$. One may then drop these subscripts and write this relation in the form of a square matrix for each positive value of k

$$\begin{pmatrix} B(k) \\ B(-k) \\ B^*(k) \\ B^*(-k) \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} S^{(1)} & S^{(2)} & S^{(3)} & S^{(4)} \\ S^{(2)*} & S^{(1)*} & S^{(4)*} & S^{(3)*} \\ S^{(3)*} & S^{(4)*} & S^{(1)*} & S^{(2)*} \\ S^{(4)} & S^{(3)} & S^{(2)} & S^{(1)} \end{pmatrix} \begin{pmatrix} A(k) \\ A(-k) \\ A^*(k) \\ A^*(-k) \end{pmatrix}. \quad (6)$$

This matrix can be reduced by splitting up the four-component vectors A and B according to

$$\begin{aligned}(A(k), A(-k), A^*(k), A^*(-k)) &= (A^{\mathrm{e}}(k), A^{\mathrm{e}*}(k), A^{\mathrm{e}*}(k), A^{\mathrm{e}}(k)) \\ &\quad +(A^{\mathrm{m}}(k), -A^{\mathrm{m}*}(k), A^{\mathrm{m}*}(k), -A^{\mathrm{m}}(k)).\end{aligned}$$

The wave packets with superscript $^{\mathrm{e}}$ are characterized by $A(-k)=A^*(k)$, so that the corresponding u is real. Hence, they represent superpositions of electric 2^l-pole waves, while A^{m} and B^{m} are magnetic 2^l-pole waves. Substitution in (6) yields

$$B^{\mathrm{e}}(k)=\tfrac{1}{2}(S^{(1)}+S^{(4)})A^{\mathrm{e}}(k)+\tfrac{1}{2}(S^{(2)}+S^{(3)})A^{\mathrm{e}*}(k), \quad (7a)$$

$$B^{\mathrm{m}}(k)=\tfrac{1}{2}(S^{(1)}-S^{(4)})A^{\mathrm{m}}(k)+\tfrac{1}{2}(S^{(2)}-S^{(3)})A^{\mathrm{m}*}(k), \quad (7b)$$

where k ranges from $-\infty$ to $+\infty$.

(e) *Conservation of Energy*

Finally, we postulate that no energy is exchanged between the radiation and the core, which according to (5) is expressed by

$$\sum_{lm}\int_{-\infty}^{+\infty}|B_{lm}(k)|^2dk=\sum_{lm}\int_{-\infty}^{+\infty}|A_{lm}(k)|^2dk.$$

In general this means that the relation between A and B is unitary, from which for the specific relation (7a) it can be inferred that either $S^{(1)}+S^{(4)}$ or $S^{(2)}+S^{(3)}$ must vanish. In the latter case

$$B^{\mathrm{e}}(k)=S^{\mathrm{e}}(k)A^{\mathrm{e}}(k), \quad |S^{\mathrm{e}}(k)|=\tfrac{1}{2}|S^{(1)}+S^{(4)}|=1.$$

One is inclined to reject the other case for the reason that there is no continuous transition to the case of no scattering possible. A better reason, however, will be given in the next section: it does not satisfy the causality condition.

The same argument applies to (7b), so that one may write for each particular electric or magnetic multipole wave

$$B(k)=S(k)A(k), \quad (-\infty<k<+\infty) \quad (8)$$

$$S(-k)=S^*(k), \quad S(k)S^*(k)=1. \quad (9)$$

It is sufficient to treat the scattering of electric multipole waves only. For the incident wave packet $A(k)$ may then be chosen any square integrable function that satisfies

$$A(-k)=A^*(k). \quad (10)$$

III. THE CAUSALITY CONDITION

For the following it is essential to assume that the core has a finite size; in other words, that there is a sphere of radius a $(0\leqslant a<\infty)$ outside of which the free-field equations are valid. Let there be an incident wave packet that is known to be rigorously zero at some large distance r_1 for all time $t<t_1$. Outgoing waves cannot be produced until this packet has reached the core; that is, not until $t=t_1+(r_1-a)$. Hence, the outgoing field at the large distance r_2 must be zero until $t=t_1+(r_1-a)+(r_2-a)$. This imposes a restriction on the S-matrix, which will be called the "causality condition" (see reference 9). It is based only on the assumptions that free wave packets do not propagate faster than light, and that they can be decomposed into ingoing and outgoing waves whose interaction is localized in the core. We proceed to investigate to what property of S it corresponds.

To avoid irrelevant complications, it is convenient to take first a point-core, so that a can be taken zero. Then the causality condition states that, if the ingoing wave packet vanishes for $t<-r$, the outgoing wave packet must vanish for $t<+r$. According to (3) or (4), the vanishing of the ingoing wave for $r+t<0$ is tantamount to $A(k)$ being the Fourier transform of a function that is zero for negative values of its argument. From this it can be concluded that $A(k)$ can be continued as a regular analytic function in the upper half of the complex k-plane, as is more precisely stated in the following mathematical theorem.[18,19]

Necessary and sufficient for a square integrable function $A(k)$ $(-\infty<k<+\infty)$ to be the Fourier transform of a function that vanishes for negative values is the existence of an analytic function $A(k+i\gamma)$ of $k+i\gamma=\lambda$ for $\gamma>0$, such that (i) $A(k+i\gamma)\to A(k)$ if $\gamma\to 0$, for almost all values of k; (ii) $A(\lambda)$ is regular for $\gamma>0$; (iii) $\int_{-\infty}^{+\infty}|A(k+i\gamma)|^2dk<M$ for $\gamma\geqslant 0$, M independent of γ. This theorem plays a central role in the present work. When we say in the following proof that a function of k is regular in the upper half-plane, we mean that it has the property described in the theorem. The abbreviations I_+, I_-, I_0 will be used to denote the upper half-plane, the lower half-plane, and the real axis.

[18] R. E. A. C. Paley and N. Wiener, *Fourier Transforms in the Complex Domain* (American Mathematical Society, New York, 1934), p. 8.

[19] E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals* (Clarendon Press, Oxford, 1937), Chapter V.

The requirement of the causality condition that the outgoing wave must vanish for $t<r$ is tantamount to $B(k)$ being the Fourier transform of a function that is zero for negative values of its argument, according to (4). Since $B(k)$ is square integrable, it can be concluded that $B(k)$ must be regular in I_+. Hence, the causality condition entails the following property of S: whenever $A(k)$ is square integrable and regular in I_+, and satisfies (10), the same is true for $S(k)A(k)$. This enables us to extend the definition of S to I_+ by putting

$$B(\lambda)=S(\lambda)A(\lambda). \quad (\lambda=k+i\gamma, \gamma>0) \tag{11}$$

Since $A(\lambda)$ and $B(\lambda)$ are analytic and regular in I_+, so is $S(\lambda)$; it cannot have poles at the zeros of $A(\lambda)$, because (11) must hold true for any $A(\lambda)$ regular in I_+. When γ goes to zero, then $A(\lambda)\to A(k)$, $B(\lambda)\to B(k)$ for almost all k, and consequently $S(\lambda)\to S(k)$ because of (8).

The definition of S can be extended to I_- by putting

$$S(k+i\gamma)=[S(k-i\gamma)]^{*-1}. \quad (\gamma<0)$$

This is a one-valued analytic function with no other singularities than poles corresponding to the zeros in I_+. For $\gamma\to 0$ it tends to $S(k)$, owing to (9). Thus, $S(\lambda)$ is defined in I_+ and in I_- and has the boundary value $S(k)$ on I_0; it then follows from the Schwarz reflection principle[20] that $S(\lambda)$ is analytic in the whole plane but for the poles in I_-.

It may be possible to prove directly that $S(\lambda)$ is bounded in I_+ by applying condition (iii) of the theorem to $B(\lambda)$. However, it is simpler to use an additional theorem,[19] which states that any function $A(\lambda)$ with the properties (i), (ii), (iii) satisfies

$$A(\lambda)=\frac{1}{2\pi i}\int_{-\infty}^{+\infty}\frac{A(k')}{k'-\lambda}dk'. \quad (\lambda \text{ in } I_+) \tag{12}$$

Choosing $A(k)=i(k+i\beta)^{-1}$ with $\beta>0$, and writing this equation (12) for the corresponding $B(\lambda)=iS(\lambda)(\lambda+i\beta)^{-1}$, one finds

$$\frac{S(\lambda)}{\lambda+i\beta}=\frac{1}{2\pi i}\int_{-\infty}^{+\infty}\frac{S(k')dk'}{(k'-\lambda)(k'+i\beta)}. \quad (\gamma, \beta>0) \tag{13}$$

Since the right-hand side is bounded for $|\lambda|\to\infty$, S cannot become infinite more strongly than $|\lambda|$. It then follows from Phragmén-Lindelöf's theorem[20] that actually S must be bounded, and even

$$|S(\lambda)|<1 \text{ for } \lambda \text{ in } I_+.$$

Incidentally, it can now be shown why the alternative possibility mentioned in Sec. II under (*e*) does not comply with the causality condition. Suppose it did; then the wave packet $A(k)=i(k+i\beta)^{-1}$ would correspond to an outgoing wave packet

$$B(k)=S(k)A(-k)=iS(k)(i\beta-k)^{-1},$$

which would be regular in I_+. Consequently, $S(\lambda)$ would be regular in I_+ with a zero at $i\beta$. This cannot be true for all $\beta>0$.

The properties of the function S may be summarized as follows. $S(\lambda)$ *is a meromorphic function, which maps the real axis onto the unit circle, the upper half-plane into the interior and the lower half-plane into the exterior; the imaginary axis is mapped onto the real axis.* We now proceed to derive from these properties a product expansion for $S(\lambda)$.

Let the zero's of $S(\lambda)$ be denoted by $\Lambda_\nu=K_\nu+i\Gamma_\nu$ $(\Gamma_\nu>0)$, so that the poles are Λ_ν^*. If the following product over all zeros,

$$\prod_\nu\frac{\lambda-\Lambda_\nu}{\lambda-\Lambda_\nu^*}, \tag{14}$$

is convergent, it is easily seen to share all the properties mentioned above for $S(\lambda)$. Dividing $S(\lambda)$ by (14) we are left with another function with the same properties, which moreover has neither zeros nor poles. It must have the form $\pm e^{-2i\alpha\lambda}$ with $\alpha\leqslant 0$ (see below), so that

$$S(\lambda)=\pm e^{-2i\alpha\lambda}\prod_\nu\frac{\lambda-\Lambda_\nu}{\lambda-\Lambda_\nu^*}. \tag{15}$$

Because of (9) the zeros Λ_ν must be symmetrical with respect to the imaginary axis. If Λ_n denotes a zero in the first quadrant $(K_n>0, \Gamma_n>0)$, then $-\Lambda_n^*$ is a zero in the second quadrant, and Λ_n^* and $-\Lambda_n$ are poles. In addition there may be unpaired zeros on the imaginary axis; they will be denoted by $iL_m (L_m>0)$, with corresponding poles $-iL_m$. Then (15) may be written

$$S(\lambda)=\pm e^{-2i\alpha\lambda}\prod_n\frac{(\lambda-\Lambda_n)(\lambda+\Lambda_n^*)}{(\lambda-\Lambda_n^*)(\lambda+\Lambda_n)}\prod_m\frac{iL_m-\lambda}{iL_m+\lambda}. \tag{16}$$

The case of an extended core can be treated in a similar way. One finds the same properties for $S(\lambda)$, except the boundedness in I_+. If the core can be enclosed in a sphere with radius a, it is found that now $e^{2ia\lambda}S(\lambda)$ must be bounded in I_+. This leads to the same expression (16), but with the weaker restriction for α

$$\alpha\leqslant a. \tag{17}$$

The constant a is only defined as an upper limit for the radius of the core and has to be guessed from some rough model. The constant α is uniquely defined, but can only be determined by actual calculation based on a specific model, or else by experiment. It plays the part of an effective radius, because on a large sphere of radius r no scattered waves are observed until a time $t=2(r-\alpha)$ after the incident wave front entered the sphere. However, it is impossible to conclude from the causality condition that negative α cannot occur.

In order to justify (16) with (17) it has to be shown that both infinite products are convergent, and that the remaining factor is necessarily of the form $\pm e^{-2i\alpha\lambda}$ with

[20] E. C. Titchmarsh, *The Theory of Functions* (Clarendon Press, Oxford, 1939), second edition.

$\alpha \leqslant a$. The criterion for the first product to be (absolutely) convergent is the convergence of the sum

$$\sum \left| \frac{(\lambda-\Lambda_n)(\lambda+\Lambda_n^*)}{(\lambda-\Lambda_n^*)(\lambda+\Lambda_n)} - 1 \right| = 4|\lambda| \sum \frac{\Gamma_n}{|(\lambda-\Lambda_n^*)(\lambda+\Lambda_n)|}.$$

Since $|\Lambda_n| \to \infty$ (the zeros cannot have an accumulation point), this depends on the convergence of $\sum \Gamma_n / |\Lambda_n|^2$. Now, by Carleman's theorem,[20] the convergence of

$$\sum \frac{\Gamma_\nu}{|\Lambda_\nu|^2} = \sum \frac{\Gamma_n}{|\Lambda_n|^2} + \sum \frac{1}{L_m} \tag{18}$$

follows from the fact that $e^{2ia\lambda}S(\lambda)$ is regular and bounded in I_+. Hence, the first product in (16) is convergent, uniformly in any finite closed region not containing a pole, so that it is a meromorphic function with poles Λ_n^* and $-\Lambda_n$. Similarly from the convergence of the last term in (18) it follows that the second product in (16) is convergent and represents a meromorphic function with poles $-iL_m$.

Now consider the function $f_N(\lambda)$, defined by

$$f_N(\lambda) = e^{2ia\lambda} S(\lambda) \Big/ \prod_{n=1}^{N} \frac{(\lambda-\Lambda_n)(\lambda+\Lambda_n^*)}{(\lambda-\Lambda_n^*)(\lambda+\Lambda_n)} \prod_{m=1}^{N} \frac{iL_m - \lambda}{iL_m + \lambda}.$$

This function is again regular and bounded in I_+ and has modulus 1 on I_0; hence, by Phragmen-Lindelöf's theorem $|f_N(\lambda)| \leqslant 1$ in I_+. As the products are convergent for $N \to \infty$, the limit $f(\lambda) = \lim f_N(\lambda)$ exists, and it can easily be seen that it has the same properties. Moreover, it has no zeros or poles, and can therefore be written $f = e^{u+iv}$, where $u+iv$ is an entire function. Its real part u is negative in I_+ and positive in I_-, so that on I_0

$$0 \geqslant \partial u/\partial\gamma = -\partial v/\partial k. \quad (\gamma=0)$$

Hence $v(k)$ increases monotonely with k and assumes any real value not more than once. Consequently, $u+iv$ assumes each purely imaginary value at most once, and must therefore be a linear function:

$$u+iv = 2i\alpha_1\lambda + \alpha_2;$$

and obviously $\alpha_1 \geqslant 0$, $\alpha_2 = 0$ or π. This completes the proof that $S(\lambda)$ has the form (16) (with $\alpha = a - \alpha_1$).

It should be noted that only the absolute convergence of the products in (16) could be proved, while the convergence of (14) may depend on the order in which the Λ_ν are numbered. (When in the following we use, nevertheless, (15), it is only meant to be a short writing for (16). Also it is not possible to conclude anything about the order of $S(\lambda)$ as a meromorphic function. The reason is that there is no other information about the density of the zeros and poles than the convergence of the Carleman sum (18), which does not prevent them from clustering about the real axis. It is remarkable that this sum is also physically important: it is the sum of the oscillator strengths, as will be shown in the next section. At this point its relation with scattering data may be established by taking the logarithmic derivative of $S(\lambda)$ at $\lambda=0$:

$$S'(0)/S(0) = 2i\{-\alpha + \sum \Gamma_\nu / |\Lambda_\nu|^2\}. \tag{19}$$

IV. PHYSICAL INTERPRETATION

The cross section for scattering can be derived from (16) by means of [21]

$$\sigma(k) = (\pi/2k^2)(2l+1)|1-S(k)|^2.$$

It may be expected that each zero Λ_n with the corresponding pole Λ_n^* will produce a resonance level. This is easily verified under the following conditions: (i) the distances Γ_n from the real axis are small compared to the mutual distances of the zero's; (ii) $\alpha K_n \ll 2\pi$ for the zero considered, i.e., the resonance wavelength is much larger than the effective radius; (iii) in (16) the $+$ sign has to be taken, i.e., $S(0)=1$. One may then write in the neighborhood of K_n

$$S(k) = \frac{k-\Lambda_n}{k-\Lambda_n^*} = \frac{k-K_n-i\Gamma_n}{k-K_n+i\Gamma_n}, \tag{20}$$

which leads to the ordinary one-level formula,

$$\sigma(k) = \frac{2\pi}{k^2}(2l+1)\frac{\Gamma_n^2}{(k-K_n)^2+\Gamma_n^2}. \tag{21}$$

When the condition (i) is not satisfied, the maximum of σ is shifted away from K_n, and the line is distorted, so that the width is no longer precisely defined. This can readily be demonstrated in the case of two overlapping lines, Λ_1 and Λ_2 say, if the other factors in (16) may again be omitted. One finds

$$\sigma(k) = \frac{2\pi}{k^2}(2l+1)\frac{\{\Gamma_1(k-K_2)-\Gamma_2(k-K_1)\}^2}{\{(k-K_1)^2+\Gamma_1^2\}\{(k-K_2)^2+\Gamma_2^2\}}. \tag{22}$$

This cross section reaches its maximum value $2\pi(2l+1)/k^2$ at the two points

$$k = \tfrac{1}{2}(K_1+K_2) \pm \tfrac{1}{2}\{(K_1^2-K_2^2)+4\Gamma_1\Gamma_2\}^{\frac{1}{2}},$$

and vanishes at $k = (\Gamma_1 K_2 + \Gamma_2 K_1)/(K_1+K_2)$. Hence, it has two peaks, whose mutual distance is never less than $\{4\Gamma_1\Gamma_2\}^{\frac{1}{2}}$. This is even true if the frequencies coincide, in which case

$$\sigma(k) = \frac{2\pi}{k^2}(2l+1)\frac{\Gamma_1+\Gamma_2}{\Gamma_1-\Gamma_2}\left\{\frac{\Gamma_1^2}{(k-K_1)^2+\Gamma_1^2} - \frac{\Gamma_2^2}{(k-K_2)^2+\Gamma_2^2}\right\}.$$

[21] $\sigma(k)$ is the total outgoing energy current in the electric (or magnetic) 2^l-pole wave, when an incident plane wave of frequency k and unit intensity is scattered. The additional factor $\frac{1}{2}$ [as compared with N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Clarendon Press, Oxford, 1933), p. 24] is related to the twofold polarization of the electromagnetic field [see N. G. van Kampen, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **26**, No. 15 (1951), Appendix B].

Thus, the total scattering owing to both coinciding levels shows up as a broad line, from which a sharper line is *subtracted* in the middle. (For the special case of equal widths ($\Gamma_1=\Gamma_2$), a slightly different expression for σ follows from (22); but physically the multiple zeros of $S(\lambda)$ may be treated as limiting cases of nearly coinciding levels.)

A similar effect is caused by any zero-pole pair sufficiently remote from the real axis. Such a pair gives rise to a broad resonance line, which forms a background for the narrow lines in the same region. The line form of both together is (22); it follows from this formula that the narrow line causes a sharp minimum and an adjoining sharp maximum in the slowly varying background.[12] The effect of the zeros iL_m can be described in the same way.

The exponential factor does not affect the scattering as long as $2\alpha k$ is sufficiently small, or near to a multiple of 2π. For lines for which $2\alpha K_n$ is not near to a multiple of 2π, but for which $2\alpha\Gamma_n$ is small, it will again act as a background, with which the resonance scattering interferes. This factor is responsible for what Bethe and Placzek[11] called "potential scattering in the narrower sense" (while potential scattering in the more general sense includes all scattering that is not due to the resonance lines in the region under consideration). An example that the exponential factor may actually occur in the electromagnetic case is furnished by Debye's calculation of the scattering by a dielectric sphere;[16] here $S(\lambda)$ is asymptotically in I_+

$$S_l(\lambda)\backsimeq(-1)^l\frac{\sqrt{\mu}-\sqrt{\epsilon}}{\sqrt{\mu}+\sqrt{\epsilon}}e^{-2ia\lambda}$$

(ϵ= dielectric constant, μ= permeability, a= radius of the sphere). However, it is due to the macroscopic treatment, and it is a fair guess that no exponential factor occurs in the scattering by a finite number of elementary particles.

The alternative minus sign in (16) cannot be ruled out on the basis of our conditions for S. It would mean that $k=0$ happens to be the center of a resonance line, for example when there is just one zero iL_1 on the real axis.

In order to describe *emission*, we choose the special wave packet

$$\begin{aligned}A(k)&=[(k-\Lambda_n^*)(k+\Lambda_n)S(k)e^{i\alpha k}]^{-1},\\ B(k)&=[(k-\Lambda_n^*)(k+\Lambda_n)e^{i\alpha k}]^{-1}.\end{aligned}\qquad(23)$$

Clearly $A(k)$ is square integrable, regular in the *lower* half-plane, and is of the type $e^{i\alpha k}$ at infinity; consequently the ingoing field vanishes for $t>-r+\alpha$. The outgoing field vanishes for $t<r-\alpha$, so that on a large sphere with radius r the total field vanishes for $-r+\alpha<t<r-\alpha$. It follows that at $t=0$ there cannot be any field in this sphere, except for the region inside the core. Hence, (23) determines a superposition of stationary scattering states that contains no radiation at $t=0$, and only outgoing radiation at $t>0$: that is an emission state. The ingoing field at $t<0$ serves to produce the desired situation at $t=0$.

The radiation field for $t>r-\alpha$ can be computed by inserting (23) in (4) and doing the integration in the complex plane:

$$F_\theta-iF_\varphi=-\frac{2}{K_nr}\left\{\frac{2\pi(2l+1)}{l(l+1)}\right\}^{\frac{1}{2}}P_l^1(\cos\theta)\times e^{\Gamma_n(r-t-\alpha)}\sin K_n(r-t-\alpha).\quad(24)$$

This is the familiar expression for a damped wave, but it should be noted that no approximations have been used in the calculation. Thus, the real parts of the zeros of $S(\lambda)$ are the exact emission frequencies, and the imaginary parts are the corresponding line widths, even when the lines overlap.

The connection of Γ_n with the usual oscillator strengths f_n can be established by comparing (24) with the result of perturbation theory. Omitting fourth and higher orders of e, one finds for the transition probability of the nth excited state of the core to the ground state, $2\Gamma_n=(2e^2K_n^2/3m)f_n$. Hence,

$$(e^2/3m)\sum f_n=\sum\Gamma_n/K_n^2,$$

which to this approximation is indeed the sum occurring in (18). Hence, an analog of the well-known sum rule exists for any scattering center complying with our general conditions; its actual value cannot be predicted, but it follows from the causality condition that it must be finite.

If Λ_n is a zero of $S(\lambda)$ with multiplicity m, it is possible to construct m different emission states by putting

$$A_{(\mu)}(k)=[(k-\Lambda_n^*)^\mu(k+\Lambda_n)^\mu S(k)e^{i\alpha k}]^{-1}.\qquad(\mu=1,2,\cdots,m)$$

The corresponding emission fields have the form (24) with additional factors $(r-t-\alpha)$. In actual physical situations it is, of course, not possible to obtain each of these line shapes separately. However, one may choose mutually orthogonal combinations of these m emission fields. They will be emitted independently, provided the excitation of the core is due to a random perturbation.[22] The energy distribution over the frequencies is then the sum of the energy distributions in the chosen orthogonal combinations—which is independent of the particular choice.

To summarize: *the S-matrix is a product of factors, each referring to one level. In emission the levels show up separately, but in the formula for the scattering cross section they all interfere in a complicated way, unless the levels are far apart.*

[22] V. Weisskopf, Z. Physik **85**, 451 (1933).

V. RELATED FUNCTIONS

The fact that $S(\lambda)$ has modulus 1 on the real axis suggests the use of a phase shift $\eta(\lambda)$, defined by

$$S(\lambda)=e^{2i\eta(\lambda)}.$$

The analytic function $\eta(\lambda)$, however, is not one-valued, but has logarithmic branch points at Λ_ν and Λ_ν^*. The imaginary part of $\eta(\lambda)$ vanishes on I_0, and if $\alpha=0$, it is positive in I_+ and negative in I_-. Hence, the derivative $\eta'(k)$ on I_0 is positive. This property makes a unique determination of η from the relation

$$\sigma(k)=(2\pi/k^2)(2l+1)\sin^2\eta(k)$$

possible, when $\sigma(k)$ is known in a certain frequency range. In the case of an extended core this is still possible, unless a is too big.

Another property of $\eta(k)$, well known for nonrelativistic particles,[23] has to be mentioned. Suppose that $\alpha=0$ and that the number of zeros and poles is finite, so that $2\eta(\lambda)$ tends to a multiple of π for $|\lambda|\to\infty$. Let there be N zeros Λ_n and M zeros iL_m. Consider the closed contour consisting of I_0 and an infinite semicircle in I_+. Since η does not vary along this semicircle and $\eta(-k)=-\eta(k)$, one has

$$\eta(\infty)-\eta(0)=\pi(2N+M). \tag{25}$$

The following generalization of (25) for the case of an infinite number of zeros can be proved: If $\eta(k)$ tends to infinity as k^ρ, then ρ is the order of the meromorphic function $S(\lambda)$; if $\eta(k)$ is bounded, the order of $S(\lambda)$ is zero.

Wigner[24] studied the mathematical properties of a matrix R, which is related to the S-matrix by

$$ikR=\frac{e^{2iak}S(k)-1}{e^{2iak}S(k)+1}=i\tan[\eta(k)+ak].$$

Actually he was concerned with the case of nonrelativistic particles and regarded R as a function of $E=k^2$. It then followed from the theory of the compound nucleus that $R(E)$ is a meromorphic function with poles only on the real axis, and maps both I_+ and I_- into themselves. We shall show that these properties follow from the causality condition, even though in the present case E has no physical meaning.

In the first place $R_1(\lambda)\equiv\lambda R(\lambda^2)$ shares all the properties of Wigner's "R-functions". Indeed, it is one-valued analytic, with poles where $e^{2ia\lambda}S(\lambda)=-1$; this equation can only be satisfied on I_0, because the left-hand side is in absolute value less than 1 in I_+, greater than 1 in I_-. Further, on drawing the vectors $e^{2ia\lambda}S(\lambda)\pm1$ in the complex plane, it is seen that the argument of $R_1(\lambda)$ is between 0 and π for $|e^{2ia\lambda}S(\lambda)|<1$, and between $-\pi$ and 0 for $|e^{2ia\lambda}S(\lambda)|>1$; which shows that $R_1(\lambda)$ maps both half-planes into themselves.

It is curious that from this fact it follows that $R(E)$—as a function of $E=\lambda^2$—is also an "R-function". Since $R_1(\lambda)$ is an R-function, it can be expanded in a Mittag-Leffler series,[24]

$$R_1(\lambda)=p\lambda+q+\sum\left(\frac{r_n}{Z_n-\lambda}-\frac{r_n}{Z_n}\right). \quad (p,\, r_n>0)$$

From this one finds a similar series for $R(E)$

$$R(E)=\frac{R_1(\lambda)-R_1(-\lambda)}{2\lambda}=p+\sum\frac{r_n}{Z^2-E},$$

which proves that it is an R-function.

Finally we mention the Mittag-Leffler series for $S(\lambda)$ itself:

$$S(\lambda)=e^{-2ia\lambda}\{c_0+\sum c_\nu/(\Lambda_\nu^*-\lambda)\}, \tag{26}$$

because it leads to the usual expression for the cross section

$$\sigma(k)=\frac{\pi(2l+1)}{2k^2}\left|\sum\frac{c_\nu}{k-K_\nu+i\Gamma_\nu}+e^{2iak}-c_0\right|^2.$$

The last two terms represent the potential scattering, but the rather arbitrary constant a is here replaced by the well-defined, though unknown, α. If the lines are far apart, then the K_n are resonance frequencies, and the widths are given by $c_n=2i\Gamma_n$. If the lines overlap, however, the connection of the quantities describing scattering with those describing emission is more involved. For a finite number of zeros and poles (26) is certainly valid (with $c_0=1$), but for an infinite number it may be divergent.

VI. INTEGRAL RELATIONS

So far the conclusions from the causality condition have been stated in terms of analytic functions, but they can be translated into relations between functions of real k only. That will give us integral equations connecting the various physical quantities. Such relations are treated in the theory of Hilbert transforms;[19] they have been used in dispersion theory[4,5] and in the theory of electric circuits.[7]

Let $\beta>\alpha$; then $e^{2i\beta\lambda}S(\lambda)\to0$ for $|\lambda|\to\infty$, $0<\arg\lambda<\pi$. Applying Cauchy's integral to a closed curve, consisting of the real axis and a semi-circle with infinite radius, one finds

$$e^{2i\beta\lambda}S(\lambda)=\frac{1}{2\pi i}\int_{-\infty}^{+\infty}\frac{e^{2i\beta k'}S(k')dk'}{k'-\lambda}. \quad (\beta>\alpha) \tag{27}$$

It should be noted that this formula expresses $S(\lambda)$—for complex λ—explicitly in $S(k)$, and therefore allows us in principle to compute the actual values of $S(\lambda)$ from experimental data. It has been remarked before[25]

[23] N. Levinson, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **25**, No. 9 (1949). There is a difference in sign, because Levinson deals with bound states of the scattered particle, rather than with resonance levels.

[24] E. P. Wigner, Ann. Math. **53**, 36 (1951).

[25] N. G. van Kampen, Phil. Mag. **42**, 851 (1951).

that this should be required when using the analytic continuation. It can only be fulfilled if there is a certain *a priori* information about the regularity and the behavior at infinity, such as supplied by the causality condition.

Let in (27) the imaginary part of $\lambda=k+i\gamma$ tend to zero. The zero of the denominator approaches the real axis and contributes a half residue; the formula becomes

$$e^{2i\beta k}S(k)=\frac{1}{\pi i}\int_{-\infty}^{+\infty}\frac{e^{2i\beta k'}S(k')}{k'-k}dk', \tag{28}$$

where it is understood that the principal value has to be taken at $k'=k$. The validity of this equation for all $\beta>\alpha$ is not only a necessary, but also a sufficient condition for the scattering to be causal outside of a sphere with radius α.

For a point-core the exponential factor in (28) cannot be dispensed with, but there is an alternative formula in which it does not occur. Since $S(\lambda)$ is bounded in I_+, one may apply Cauchy's integral to $S(\lambda)/\lambda$, provided the pole at $\lambda=0$ is taken into account

$$\frac{S(\lambda)}{\lambda}=\frac{1}{2\pi i}\int_{-\infty}^{+\infty}\frac{S(k')dk'}{k'(k'-\lambda)}+\frac{S(0)}{2\lambda} \tag{29}$$

(principal value at $k'=0$). This is an alternative for (27); by taking λ real one finds in place of (28):

$$S(k)-S(0)=\frac{k}{\pi i}\int_{-\infty}^{+\infty}\frac{S(k')}{k'(k'-k)}dk'$$

(principal value at $k'=0$ and at $k'=k$). Separating real and imaginary parts

$$\begin{aligned}\mathcal{I}S(k)&=-\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathcal{R}S(k')}{k'(k'-k)}dk'=-\frac{2k}{\pi}\int_{0}^{\infty}\frac{\mathcal{R}S(k')}{k'^2-k^2}dk'\\ \mathcal{R}S(k)&=S(0)+\frac{2k^2}{\pi}\int_0^\infty\frac{\mathcal{I}S(k')}{k'(k'^2-k^2)}dk'.\end{aligned} \tag{30}$$

These relations have been mentioned in a paper by Jost, Luttinger, and Slotnick[26] and have been used by Rohrlich and Gluckstern[27] for the calculation of forward Delbrück scattering. To justify its application, however, the causality condition has to be postulated.

[26] Jost, Luttinger, and Slotnick, Phys. Rev. **80**, 189 (1950).

[27] F. Rohrlich and R. L. Gluckstern, Phys. Rev. **86**, 1 (1952). Actually they deal with inelastic scattering, which we hope to treat in another paper.

The above relations can be used to write the sum rule (19) in a new form. One finds first from (19)

$$\begin{aligned}\sigma(0)&=\tfrac{1}{2}\pi(2l+1)|S'(0)|^2\\ &=2\pi(2l+1)\{-\alpha+\sum\Gamma_\nu/|\Lambda_\nu|^2\}^2,\end{aligned}$$

provided $S(0)=1$. It then follows from (30) for the case of a point-core ($\alpha\leqslant 0$) that

$$\begin{aligned}\int_0^\infty\sigma(k)dk&=\pi^{\frac{3}{2}}[(l+\tfrac{1}{2})\sigma(0)]^{\frac{1}{2}}\\ &=\pi^2(2l+1)\{-\alpha+\sum\Gamma_\nu/|\Lambda_\nu|^2\}.\end{aligned} \tag{31}$$

Without restriction to a point-core one finds

$$\sum\Gamma_\nu/|\Lambda_\nu|^2=\frac{2}{\pi}\int_0^\infty\sin^2(\eta+\alpha k)\frac{dk}{k^2}.$$

A new sum rule can be derived by integrating

$$\int\{1-S(\lambda)e^{2i\alpha\lambda}\}d\lambda$$

along the same closed contour. There is no pole, but the contribution of the large semi-circle is no longer zero. If the number of zero's is finite, then for $|\lambda|\to\infty$

$$e^{2i\alpha\lambda}S(\lambda)=\prod(1-\Lambda_\nu/\lambda)(1-\Lambda_\nu^*/\lambda)^{-1}\simeq 1-(2i/\lambda)\sum\Gamma_\nu,$$

and the integration yields

$$2\pi\sum\Gamma_\nu=\int_0^\infty|1-e^{2i\alpha k}S(k)|^2dk,$$

which for $\alpha=0$ takes the simple form

$$\int_0^\infty k^2\sigma(k)dk=\pi^2(2l+1)\sum\Gamma_\nu. \tag{32}$$

For non-overlapping lines this equation is a trivial consequence of (21). If there are infinitely many lines, (32) may become meaningless, in contrast to (31). Both (31) and (32) lead to the same average cross section over a region large enough to contain many lines, but small compared to the frequency, viz.,

$$\bar{\sigma}(k)=(\pi/k)^2(2l+1)\bar{\Gamma}(k).$$

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