

CAN THE S-MATRIX BE GENERATED FROM ITS LOWEST-ORDER TERM?

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Synopsis

The suggestion that the S -matrix can be generated from its lowest-order term by successive applications of the unitarity and causality conditions, is tested on a simple example. It is shown that the procedure is vitiated by the breakdown of the expansion near resonance, which makes an application of the Kramers-Kronig relations to the separate terms impossible. In the case of propagation of waves through a medium the state of affairs is analogous.

1. *The generating procedure for the construction of S .* It has repeatedly been suggested that it should be possible to generate the whole S -matrix by computing only its lowest-order term in the coupling constant, and using the unitarity and causality conditions to find the higher terms. The suggested procedure is as follows. Suppose S may be expanded in powers of some parameter ε , which is usually the coupling constant (or rather its square),

$$S = 1 + \varepsilon S_1 + \varepsilon^2 S_2 + \dots, \quad (1)$$

and let S_1 be known, for instance by some second-order perturbation calculation. The unitarity condition reads

$$1 \equiv S^* S = 1 + \varepsilon(S_1 + S_1^*) + \varepsilon^2(S_2 + S_2^* + S_1^* S_1) + \dots, \quad (2)$$

which implies that the coefficients of ε , ε^2 , ... must vanish. Consequently the real part of S_2 is uniquely determined by S_1 . From the causality condition it follows that S satisfies the two Kramers-Kronig relations, which express the imaginary part of S in the real part and *vice versa*. Hence the imaginary part of S_2 can be found as soon as the real part is known, so that S_2 is completely determined by S_1 . It is easily seen that the procedure may be continued to yield successively the higher terms S_3 , S_4 , ...

Irrespective of the question whether this procedure is useful in actual calculations, it does show that the lowest order scattering embodied in S_1 determines all higher orders. This surprising result is, in fact, paradoxical, as is made clear by the following example. Suppose that the total Hamiltonian

has the form

$$H = H_0 + \varepsilon H_1 + \varepsilon^2 H_2.$$

Then the lowest-order scattering only involves H_1 and is independent of H_2 . Consequently the whole S -matrix would be independent of H_2 .

This argument is not entirely conclusive, because it might be so that, if a Hamiltonian is of this type, the causality condition uniquely determines H_2 when H_1 is known. However, it is easy to construct examples to show that this cannot be the case. The simplest example is obtained by putting $\varepsilon = \varepsilon'(1 + c\varepsilon')$ where c is some numerical constant. This amounts to

$$H = H_0 + \varepsilon' H_1 + \varepsilon'^2 (cH_1 + H_2).$$

Now S may be expanded as a power series either in ε or in ε' . Since the first coefficients in both expansions are identical, all the coefficients must be identical. Hence

$$S(\varepsilon) = S(\varepsilon + c\varepsilon^2)$$

for every c , which can only be true if S does not depend on ε at all.

The only escape from this paradox is a failure of the procedure outlined in the first paragraph. It is the object of this note to demonstrate by means of a simple example that such is indeed the case. The point is, that *although S satisfies the causality condition, each individual expansion coefficient in (1) does not*. In fact, the coefficients S_1, S_2, \dots , considered as functions of e.g. the energy of the incident particle, have poles on the real axis of increasingly high degrees, which make an application of the Kramers-Kronig relations spurious.

Actually this could have been expected from the outstart. Suppose that a field is scattered by a fixed scatterer, and that the latter has an eigenfrequency ω_0 . Then there will be a resonance peak with a certain width γ , which corresponds to a pole of S at $\omega_0 - i\gamma$ ¹⁾. More precisely, such a resonance is connected with a factor 2)³⁾

$$\frac{\omega - \omega_0 - i\gamma}{\omega - \omega_0 + i\gamma} = 1 - \frac{2i\gamma}{\omega - \omega_0 + i\gamma} \quad (3)$$

in the function $S(\omega)$, where ω is the frequency of the incident field. When the coupling constant tends to zero, ω_0 does not change, whereas γ also tends to zero, because it measures the probability of emission and absorption. Hence γ is at least of first order in the coupling constant, so that the expansion of (3) is

$$1 - \frac{2i\gamma}{\omega - \omega_0} - \frac{2\gamma^2}{(\omega - \omega_0)^2} + \frac{2i\gamma^3}{(\omega - \omega_0)^3} - \dots$$

It thus appears that in S_1 the resonance shows up as a pole on the real axis, because the damping term in the denominator is of higher order. It is also seen that the higher terms contain poles of increasing degree at the same point $\omega = \omega_0$.

Our conclusion is, that *the generating procedure breaks down, because the expansion (1) of S is not valid near resonance* *). Therefore the Kramers-Kronig relations cannot be applied to the separate terms of the expansion, as they involve an integration over the whole range of frequencies.

2. *The procedure tested on a special model.* In this section a special example is worked out to demonstrate the state of affairs described in section 1. For the field that is going to be scattered we take a real field $u(\mathbf{r}, t)$ satisfying the wave equation

$$\nabla^2 u - \ddot{u} = 0 \quad (4)$$

(neutral mesons of zero mass). It is essential to have zero mass, because otherwise the Kramers-Kronig relations do not apply. For the scatterer we take a harmonic oscillator with proper frequency ω_0 . To avoid complications this oscillator is supposed spherically symmetrical and should be visualised as a source or sink of oscillating strength. The interaction is localised at the origin and must be bilinear, because otherwise one cannot hope to find an exact solution of the scattering problem. We are thus led to the Hamiltonian

$$H = \frac{1}{2}(P^2 + \omega_0^2 Q^2) + eQ\tilde{u} + \frac{1}{2} \int \{v^2 + (\nabla u)^2\} d\mathbf{r}. \quad (5)$$

Here P, Q are canonical variables for the oscillator, and $v(\mathbf{r}), u(\mathbf{r})$ for the field. e is the coupling constant, and \tilde{u} denotes the value of $u(\mathbf{r})$ at the origin. Actually, if there is a point source at the origin, u has a singularity of the type $1/r$; hence one must attribute a small extension to the source,

$$e\tilde{u} = \int \varrho(\mathbf{r}) u(\mathbf{r}) d\mathbf{r}.$$

Concerning the "source density" ϱ it is only necessary to require that it is a smooth function whose extension is small compared to the wave length $1/\omega_0$ of the resonance radiation †).

This model is very similar to the non-relativistic dipole approximation for the interaction of the electron with the electromagnetic field, which was used by Pauli and Fierz ⁴⁾ and by Kramers ⁵⁾. It has been modified, however, in such a way that everything is spherically symmetric, so that polarization does not come in.

* In other words, the effect of damping cannot properly be taken into account by an expansion in the coupling constant. This, of course, has been known ever since Lorentz' theory of the electron.

† It is possible to work out the S -matrix exactly for an arbitrary $\varrho(\mathbf{r})$, but the discussion is rather complicated.

It is possible to reduce (5) by successive canonical transformations to a sum of oscillators, after which the solution of the scattering problem is trivial ⁶⁾. However, we prefer to work directly on the equations of motion, which follow from (5):

$$\begin{aligned} \dot{Q} &= P, & \dot{P} &= -\omega_0^2 Q - e\tilde{u}, \\ \dot{u}(\mathbf{r}) &= v(\mathbf{r}), & \dot{v}(\mathbf{r}) &= \nabla^2 u(\mathbf{r}) - Q\varrho(\mathbf{r}). \end{aligned}$$

For stationary solutions with a time factor $e^{-i\omega t}$ these equations simplify to

$$(\omega^2 - \omega_0^2) Q = e\tilde{u}, \quad (6)$$

$$(\nabla^2 + \omega^2) u(\mathbf{r}) = Q\varrho(\mathbf{r}). \quad (7)$$

Outside the scatterer u satisfies (4) and may be expanded in multipole waves. Only the monopole wave interacts with the scatterer, so that it involves a phase shift $\eta(\omega)$:

$$u(\mathbf{r}, t) = r^{-1} \sin(\omega r + \eta) e^{-i\omega t}. \quad (8)$$

Supposing that the extension of the source is small compared to the wave length, one finds

$$e\tilde{u} = e\omega \cos \eta e^{-i\omega t} + \int r^{-1} \varrho(\mathbf{r}) \, d\mathbf{r} \sin \eta e^{-i\omega t}. \quad (9)$$

For the integral we write e/r_0 , where r_0 is some positive number depending only on the "structure" of the point source.

In order to deal with (7) we integrate it over the source and substitute for u the monopole wave (8)

$$\begin{aligned} eQ &= \int (\nabla^2 + \omega^2) u(\mathbf{r}) \, d\mathbf{r} \\ &= e^{-i\omega t} \int (\nabla^2 + \omega^2) (r^{-1} \sin \omega r \cos \eta + r^{-1} \cos \omega r \sin \eta) \, d\mathbf{r} \\ &= e^{-i\omega t} \int -4\pi \delta(\mathbf{r}) \sin \eta \, d\mathbf{r} \\ &= -4\pi \sin \eta e^{-i\omega t}. \end{aligned}$$

Inserting this result and (9) into (6) one obtains a relation for $\eta(\omega)$:

$$\tan \eta(\omega) = \frac{e^2}{4\pi} \frac{\omega}{\omega_0^2 - \omega^2 - (e^2/4\pi r_0)}. \quad (10)$$

Since the stationary scattering states have now been found, the S-matrix is also known. It is diagonal in the multipole-wave representation and all diagonal elements are unity excepting the first one, which is according to (10)

$$S(\omega) = e^{2i\eta(\omega)} = \frac{\omega^2 - \omega_0^2 + \varepsilon/r_0 - i\varepsilon\omega}{\omega^2 - \omega_0^2 + \varepsilon/r_0 + i\varepsilon\omega}, \quad (11)$$

where $\varepsilon = e^2/4\pi$. It is evidently unitary, holomorphic and bounded in the

upper half of the complex ω -plane (including the real axis), tends to 1 at infinity, and has two simple poles in the lower half plane.

Expanding in powers of ε ,

$$S(\omega) = 1 + \varepsilon \frac{-2i\omega}{\omega^2 - \omega_0^2} + \varepsilon^2 \frac{-2\omega^2 + 2i\omega/\nu_0}{(\omega^2 - \omega_0^2)^2} + \dots \quad (12)$$

It is clear that the real part of S_2 could indeed have been determined by using (2), since one has according to (12)

$$S_2 + S_2^* = -4\omega^2/(\omega^2 - \omega_0^2)^2 = -|S_1|^2. \quad (13)$$

On the other hand it is clear that the imaginary part of S_2 cannot be found from the real part, because it contains the independent quantity ν_0 , which determines the shift of the resonance frequency due to the interaction (Lamb shift). In fact, the Kramers-Kronig relation for the S-matrix³⁾

$$\text{Im } S(\omega) = -\frac{2k}{\pi} \int_0^\infty \frac{\text{Re } S(\omega')}{\omega'^2 - \omega^2} d\omega'$$

is meaningless when applied to S_2 , owing to the double pole in (13).

3. *Supplementary remarks.* In the paper by Jost, Luttinger, and Slotnick⁷⁾ the generating procedure is formulated in a somewhat different way, which at first seems to apply to functions of the type of S_2 . They state that if a function is holomorphic everywhere but for poles on the real axis, and if this function vanishes at infinity, then it is uniquely determined by the values of its real part on the real axis. However, this statement can easily be disproved by considering the family of functions

$$iz^{-m} P_{m-1}(z), \quad (m = 1, 2, \dots) \quad (14)$$

where $P_{m-1}(z)$ is any polynomial of degree $m - 1$ with real coefficients. Although these functions have the same real part on the real axis (namely zero), and satisfy the requirements, they contain many arbitrary coefficients. The imaginary part of S_2 , as given by (12), is just such a function, which explains why it can contain a constant that is not contained in the real part. In general, S_m has a pole of degree m at $\omega = \omega_0$, so that its imaginary part is determined by its real part, apart from an arbitrary term of the form (14), involving $m - 1$ arbitrary real constants.

As a second example we consider the propagation of light through a medium. A plane wave is described by the expression

$$e^{i\omega n z - i\alpha x - i\omega t} = e^{i\omega n z - i\omega t}.$$

Here $\mathbf{n}(\omega) = n(\omega) - i\alpha(\omega)/2\omega$ is the complex refractive index, and the

velocity of light in vacuo is 1. The model of Lorentz gives for $\mathbf{n}(\omega)$

$$\mathbf{n}(\omega) - 1 = 2\pi \sum \frac{N_j f_j e^2/m}{\omega_j^2 - \omega^2 + i(2\omega_j^2 f_j e^2/3m)\omega}. \quad (15)$$

This equation determines both $\mathbf{n}(\omega)$ and $\alpha(\omega)$ in terms of the constants that describe the medium, and is therefore analogous to the explicit expression (11) for $S(\omega)$. The lowest-order approximation to (15) is Sellmeier's formula

$$\mathbf{n}(\omega) - 1 = 2\pi \sum_j N_j f_j e^2/m(\omega_j^2 - \omega^2). \quad (16)$$

Obviously one cannot hope to generate (15) from (16), because (16) is invariant for a change of N_j and f_j with fixed product $N_j f_j$, whereas (15) is not.

In this connection a remark on the difference between a *Kramers-Kronig relation* and a *dispersion formula* may be added. The refractive index and the absorption coefficient are *connected* by the Kramers-Kronig relation ⁸⁾

$$\mathbf{n}(\omega) - 1 = \frac{1}{\pi} \int_0^\infty \frac{\alpha(\omega')}{\omega'^2 - \omega^2} d\omega'. \quad (17)$$

This relation is equivalent to the statement that $\mathbf{n}(\omega)$ is holomorphic in the upper half of the complex ω -plane (and satisfies certain conditions at infinity). There is of course a wide variety of such functions, so that (17) does not at all determine $\mathbf{n}(\omega)$ and $\alpha(\omega)$, but only restricts the possibilities. On the other hand, the *dispersion formula* (15) gives a specific expression for both $\mathbf{n}(\omega)$ and $\alpha(\omega)$, so that they are fully known, if the medium is known. Of course, the \mathbf{n} and α given by this dispersion formula obey the condition (17) (because the right-hand side of (15) is holomorphic in the upper half plane, including the real axis, and tends to zero at infinity). But (15) is *not* a consequence of (17); indeed, it is easy to construct a dispersion formula that cannot be written in the form (15) and yet obeys (17); e.g.,

$$\mathbf{n}(\omega) - 1 = (\omega + i)^{-1} e^{i\omega}.$$

The regrettable fact that the Kramers-Kronig relations are at present usually referred to as "dispersion relations" tends to obscure this fundamental difference between a specific dispersion formula, and the general condition provided by the Kramers-Kronig relations. It seems to me that an insufficient understanding of this difference is responsible for the opinion that "dispersion relations" may ultimately take the place of field theory. Indeed, the theory of the electromagnetic field in media has not been replaced by the equation (17), nor has mechanics been made superfluous by the law of conservation of energy.

Another circumstance adds to the confusion. Sellmeier's dispersion formula (16) is not only an approximation to (15), but also shows a remarkable similarity to the Kramers-Kronig relation (17). Although this similarity

led both Kronig and Kramers to the discovery of (17), it is deceptive. It happens to be true that (16) can be obtained as a special case of (17) by putting

$$\alpha(\omega) = 2\pi^2 \sum_j (N_j f_j e^2/m) \delta(\omega - \omega_j),$$

but this only works owing to the omission of the damping term. The full dispersion formula (15) cannot be obtained from (17) by any special choice of $\alpha(\omega)$; in fact, it is quite differently constructed, as it expresses the equality of two *complex* quantities, one of which contains n and α , while the other only refers to properties of the medium.

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REFERENCES

- 1) Møller, C., Dan. mat. fys. Med. **22** (1946) no. 19.
- 2) Hu, N., Phys. Rev. **74** (1948) 131; Heisenberg, W., *Theorie des Atomkerns* (Göttingen 1951).
- 3) Van Kampen, N. G., Phys. Rev. **89** (1953) 1072.
- 4) Pauli, W., and Fierz, M., Nuovo Cimento **15** (1938) 167.
- 5) Kramers, H. A., Report Solvay Congress 1948; *Collected Scientific Papers* (Amsterdam 1956), p. 845.
- 6) Van Kampen, N. G., Dan. mat. fys. Med. **26** (1951) no. 15; Steinwedel, H., Fortschritte Phys. **1** (1953) 7; Steinwedel, H., Ann. Physik (6) **15** (1955) 207; McVoy, K., and Steinwedel, H., Nuclear Physics **1** (1956) 164.
- 7) Jost, R., Luttinger, J. M., and Slotnick, M., Phys. Rev. **80** (1950) 189.
- 8) Kronig, R., J. opt. Soc. America **12** (1926) 547; Kramers, H. A., Nature **117** (1926) 775; Atti cong. intern. fisici (Como 1927) **2**, 545; Phys. Z. **30** (1929) 522; *Collected Scientific Papers* (Amsterdam 1956), p. 333 and p. 347; J. S. Toll, Thesis (Princeton 1952).