THE CONNECTION BETWEEN THE R-MATRIX AND THE S-MATRIX.

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RESUMEN

It is shown that the analytic properties that Wigner found for the R-matrix are equivalent with the properties of the S-matrix that can be deduced from the causality condition.

I. Introduction.

The present note deals with elastic scattering of non-relativistic Schrödinger particles by a fixed centre. The scattering centre is supposed to be of finite size, so that it can be enclosed in a sphere with radius a. For simplicity we assume spherical symmetry and consider only S-waves. The scattering can then be completely described either by the

"S-matrix" (which in this case reduces to a scalar function of p), or by the "R-matrix", which is related to S by

$$e^{2iap}\, S(p) = \frac{1+ip\, R(p^2)}{1-ip\, R(p^2)} \quad . \qquad (1)$$

p is the magnitude of the momentum of the incident particle and p^2 is its energy, the mass being taken equal to $\frac{1}{2}$.

Wigner[1] showed that if the interaction inside the scattering centre can be described by a self-adjoint operator, the function R(w) has the following properties:

(a) R(w) is a meromorphic function of $w = u+iv$;

(b) R(u) is real;

(c) All poles of R lie on the real axis;

(d) The imaginary part of R is positive in the upper half plane and negative in the lower half plane.

According to a theorem of Herglotz[2] one can conclude quite generally from this that the following expansion is valid

$$R(w) = \alpha w + \beta + \Sigma \left\{ \frac{\gamma_n^2}{u_n - w} - \frac{\gamma_n^2}{u_n} \right\} , \qquad (2)$$

where the constants $\alpha, \beta, \gamma_n, u_n$ are real and $\alpha \geqslant 0$. The poles u_n may approach infinity in both directions but cannot accumulate in a finite point. Wigner and Eisenbud[3] showed that actually

$$R(w) = \Sigma \frac{\gamma_n^2}{u_n - w} \qquad , \qquad (3)$$

which amounts to adding one more property:

(e) The sum $\Sigma(\gamma_n^2/u_n)$ converges and equals β, and $\alpha = 0$

The question arises to what properties of S these properties (a) - (e) of R correspond. From (1) in connection with (a) and (b) follow immediately

(a') S(z) is a meromorphic function of $z = x+iy$;

(b') On the real axis is

$$S(x)^{-1} = S(x)^* = S(-x) \quad . \tag{4}$$

Schützer and Tiomno[4] showed that (d) implies

(c') The poles of S lie either on the positive imaginary axis or in the lower half plane.

In a recent paper[5] Wigner deduced some properties of S from (a) - (d), but they were not yet sufficient to prove conversely the properties of R. On the other hand it has been shown[6] that the so-called causality condition entails the following additional properties of S:

(d') In the first quadrant of the z-plane

$$\text{Img } e^{2ias} S(z) \leqslant 1 \quad ; \tag{5}$$

(e') $e^{2ias} S(z)$ is bounded in $0 \leqslant \text{Arg } z \leqslant \frac{\pi}{2} - \delta$.

It was also shown that (a') - (e') are sufficient to derive (a) - (d).

In the present note we intend to demostrate firstly that (a') - (e') also imply (e), and secondly that (a) - (e) imply (d') and (e') The result can be stated in the following theorem: <u>The properties (a) - (e) for R are equivalent with the properties (a') - (e') for S.</u> It can readily be verified that the properties that Wigner[5] deduced for S are contained in (a′) – (e′).

II. (a′) – (e′) imply (e)

With the abbreviation $e^{2iaz} S(z) = S_a(z)$, (1) gives

$$R(z^2) = \frac{1}{iz} \frac{S_a(z)-1}{S_a(z)+1} \qquad (6)$$

It follows that R(w) on the imaginary axis tends to zero:

$$R(iv) = O(v^{-\frac{1}{2}}) \quad , \qquad (7)$$

unless $S_a(re^{\pi i/4})$ tends to -1 for $r \to \infty$. To exclude this eventuality we shall suppose that a is chosen slightly larger than the radius of the smallest sphere in which the scattering centre can be enclosed. Then we know that there is a small ϵ such that $e^{2i(a-\epsilon)z} S(z) = e^{-2i\epsilon z} S_a(z)$ is bounded, and therefore that certainly $S_a(re^{\pi i/4}) \to 0$. Hence for such a choice of a the validity of (7) is guaranteed.

Now consider the imaginary part of R(iv) as given by (2)

$$\text{Img } R(iv) = \alpha v + v\Sigma \frac{\gamma_n^2}{u_n^2 + v^2} \quad .$$

Clearly $\text{Img } R(iv)/v \to \alpha$ as $v \to \infty$, so that from (7) follows $\alpha = 0$. Next we have[7]

$$\int_0^\infty \frac{\operatorname{Img} R(iv)}{v}\, dv \geq \int_0^\infty \sum_{-N}^{+M} \frac{\gamma_n^2}{u_n^2+v^2}\, dv = \frac{\pi}{2}\sum_{-N}^{+M} \frac{\gamma_n^2}{|u_n|} .$$

As the left side converges owing to (7), the sum on the right is bounded when M and N tend to infinity One may therefore write

$$R(w) = \left[\beta - \Sigma \frac{\gamma_n^2}{u_n} \right] + \Sigma \frac{\gamma_n^2}{u_n - w} ;$$

since both the left side and the last term on the right tend to zero as $w \to i\infty$, the constant term [ ] must be zero, so that (3) is proved.

For this proof it was assumed that $R(w)$ is defined with a value of a which is slightly higher than the lowest value for which (5) is true. That this cannot be avoided is shown by the example

$$S(z) = \frac{i-z}{i+z} .$$

Clearly this S satisfies (a') - (e') with $a = 0$. However if one defines R by taking $a = 0$ in (6), it becomes identically 1; this R satisfies (a) - (d) and is of the form (2), but cannot be written in the form (3).

III. <u>(a) - (e) imply (d')</u>

We first assume that R is given by an expression (3) with a finite number of terms. Then both R and S_a are rational functions and as $R(z^2) = O(z^{-2})$ one has

$$\lim S_a(z) = 1 \quad \text{for} \quad |z| \to \infty \ .$$

From (4) one sees that

$$S_a(-z^*) = S_a(z)^* \quad ,$$

and therefore that $S_a(z)$ is real on the imaginary axis. Hence $\operatorname{Img} S_a$ vanishes on the imaginary axis and at infinity and satisfies (5) on the real axis; since it is a harmonic function in the first quadrant its maximum must lie on the boundary, so that (5) is indeed satisfies in the whole quadrant. To make this proof rigorous, however, we have to consider more carefully what happens in the neighbourhood of the poles on the imaginary axis.

These poles are the points iy for which

$$yR(-y^2) + 1 = 0 \ , \qquad y > 0 \ .$$

It follows from (d) and is obvious from (3) that $R'(u) > 0$ and hence that in each of these points

$$\frac{d}{dy} \{ yR(-y^2) + 1 \} = R(-y^2) + y \frac{d}{dy} R(-y^2)$$

$$= -\frac{1}{y} - 2y^2 \frac{d}{du} R(u)$$

is negative. Consequently the residue of $S_a(z)$ at each pole $i\kappa_n$ is $-ic_n$ with $c_n > 0$:

$$S_a(z) = \frac{-ic_n}{z - i\kappa_n} + g(z) \quad , \qquad (8)$$

where $g(z)$ is regular in the neighbourhood and again real on the imaginary axis. This shows that it is possible to draw a small semicircle in the first quadrant about the pole, on which $\operatorname{Img} S_a(z) \leq 0$. Hence the use of the maximum modulus principle was indeed justified.

Now consider an R given by (3) with an infinite number of terms. We can then first form a mutilated R by taking only N terms of the series and the above proof shows that (5) holds for the corresponding mutilated S. If then $N \to \infty$ it is clear that (5) must also hold for the limiting S.

IV. (a) - (e) imply (e')

We first establish the preliminary estimate

$$S_a(z) = o(|z|^2) \quad \text{as} \quad |z| \to \infty, \quad 0 \leq \operatorname{Arg} z \leq \frac{\pi}{2} - \delta. \qquad (9)$$

According to Herglotz's theorem[2] one may express the values of the function $i-S_a(z)$ in terms of a Poisson-Stieltjes integral, taken along the boundary of the first quadrant. That gives

$$i-S_a(z) = \alpha' z^2 + \beta' + \Sigma \left\{ \frac{\gamma_n'^2}{u_n'-z^2} - \frac{\gamma_n'^2}{u_n'} \right\} +$$

$$+ \frac{2}{\pi} \int_0^\infty \frac{1+\xi^2 z^2}{\xi^2-z^2} \, \frac{1-\operatorname{Img} S_a(\xi)}{1+\xi^4} \, \xi \, d\xi \qquad (10)$$

This equation is the analog of (2), but an integral now also appears on the right, owing to the fact that $S_a(z)$ is not real on the positive real axis. As there are no poles for real z, all u_n' are negative, say $u_n' = -\kappa_n^2 (\kappa_n > o)$. Comparison with (8) yields $\gamma_n'^2 = +2\kappa_n c_n$. After some manipulations (10) becomes

$$\frac{S_a(z) - S_a(o)}{z} + 2z \, \Sigma \frac{c_n}{\kappa_n(\kappa_n^2 + z^2)} = -\alpha' z + \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Img } S_a(\xi)}{\xi(\xi - z)} d\xi \, .$$

The right-hand side is a function that is regular in the whole upper half plane and of order $|z|$ as $|z| \to \infty$. The left side shows that on the real axis it is of order less than $|x|$. According to the theorem of Phragmén and Lindelöf[8] it must therefore be of order less than $|z|$ in the whole upper half plane. From this follows (9), because the sum in the second term on the left vanishes if z tends to infinity in the angle between 0 and $\frac{\pi}{2} - \delta$. It also follows that $\alpha' = 0$.

Now consider the function

$$S_b(z) = e^{2ibs} \, S(z) = e^{2i(b-a)s} \, S_a(z)$$

with $b \geqslant a$. Clearly $S_b(z)$ satisfies (a′) – (c′), so that $\text{Img } S_b(z) \leqslant 1$ on the boundaries of the first quadrant. Moreover in the first quadrant it is not greater in absolute value than $S_a(z)$, so that

$$S_b(z) = o(|z|^2) \, , \qquad 0 \leqslant \text{Arg } z \leqslant \frac{\pi}{2} - \delta \quad .$$

Hence one can apply Phragmén-Lindelöf's theorem to

$$F(z) = \exp i\, S_b(z)$$

with the result that $|F(z)| \leqslant e$ and therefore

$$\operatorname{Img} S_b(z) \leqslant 1 \qquad (11)$$

in the whole quadrant.

One can now find a bound for $|S_a(z)|$ from (11) by choosing a suitable value for b. Let for a fixed z

$$S_a(z) = |S_a|\, e^{i\Phi} \quad ,$$

so that (11) becomes

$$e^{-2(b-a)y}\, |S_a| \sin\{2(b-a)x + \Phi\} \leqslant 1 \;. \qquad (12)$$

It is certainly possible to choose a $b \geqslant a$ such that

$$\sin\{2(b-a)x + \Phi\} = 1 \quad , \qquad b-a < \pi/x \;.$$

With this choice (12) becomes

$$|S_a(z)| \leqslant e^{2\pi(y/x)} \;,$$

which proves (e').

Appendix

Wigner and Eisenbud[3] introduce the set of solutions $X_\lambda(r)$ of the Schrödinger equation, satisfying $X_\lambda'(a) = 0$, and expand an arbitrary solution $\varphi(r)$ in the form

$$\varphi(r) = \Sigma A_\lambda X_\lambda(r) \quad . \qquad (0 \leq r < a)$$

For the proof of (3) it is essential that this expansion should also hold for $r = a$, which is not obvious. However, it can readily be proved when the interaction is given by a potential field $V(r)$. Indeed, if $V = 0$ the validity follows from the theory of Fourier series, and it is known that the presence of a potential field does not influence the convergence[9]. Actually, in the case of a potential field, (3) can be proved more directly by using the asymptotic expressions[9]

$$\varphi(p,r) \simeq \sin pr/p \quad , \qquad \varphi'(p,r) \simeq \cos pr \quad ,$$

for $p \to i\infty$, which give

$$R(p^2) \simeq \tan pa/p = O\left(\frac{1}{p}\right) \quad ;$$

according to the proof in section II this entails (3).

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2. See e.g. M.H.Stone, Linear Transformations in Hilbert Space (New York 1932) p. 570. This theorem states essentially that if the imaginary part of an analytic

function is non-negative in a certain region, the functic can be expressed in terms of the boundary values of its imaginary part by means of a Poisson-Stieltjes integral.
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7. For this proof I am indebted to Professor H. Pollard.
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