Chapter 3

ANALYTICAL PROPERTIES OF THE WAVE FUNCTION

§ 13. ANALYTICAL PROPERTIES OF THE *S*-MATRIX

In the preceding chapter we showed that the scattering of particles in a potential field is completely described by the phase factors $S_l(k) = \exp(2i\delta_l(k))$.

If we know the exact form of the particle interaction potential, analytical or numerical solution of the Schroedinger equation will provide complete information on the system. Had this always been the case, we could leave with free conscience all the problems of quantum mechanics to electronic computers, and proceed with matters of more importance. However, the actual physical reality is far from this ideal state of things. In most cases, the particle interaction potential is simply not known. Moreover, the actual interaction between particles is apparently not described by potential forces.

Non-potential interactions are the subject of what is called quantum field theory. (Simple problems of this kind are considered in Chapter 8.) This theory, however, unlike quantum mechanics, is not free from internal difficulties. For example, calculation of certain quantities involves divergences (infinite, unbounded results). These divergences are apparently associated with improper description of interaction at very small distances.

Heisenberg /83/ attributed these difficulties to the use of nonobservables, such as $\psi(r)$, in the theory; a proper theory should deal only with observables, which include the functions $S_l(k) = \exp(2i\,\delta_l(k))$ forming the so-called *S* matrix (scattering matrix) /84/. The theory of the *S*-matrix is rapidly developing in recent years, especially in connection with the description of strong interactions of elementary particles. Particular attention is devoted to the construction of *S*-matrix theory using unitarity and analyticity properties. (Note that the importance of the analytical properties of the *S*-matrix was first emphasized by Kramers /85/ and Heisenberg /86/.) Numerous important advances were accomplished in this direction and various relations between experimental observables were established. Thus, the considerable progress in the theory of elementary particles is definitely attributed to ingenious application of the analytical properties of the *S*-matrix. Moreover, in case of quasistationary states and in some other cases, the behavior of a system can be described without introducing a particular interaction: it suffices to apply only general considerations on the position of the poles of the scattering amplitude.

The *S*-matrix formalism is generally regarded as precluding space-time description of processes. We should stress at this point that recent results /87, 88/ give actual prescriptions for space-time separation of

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events within the framework of the *S*-matrix formalism. The applicability of intensity correlations to the determination of the scattering amplitude phase was demonstrated in /89–91/.

We will discuss the analytical properties of functions proceeding from the following general considerations:

(a) all the energy eigenvalues are real (a Hermitian Hamiltonian); the wave vector k is thus automatically real for continuum wave functions;

(b) elastic scattering is the only allowed process;

(c) the Hamiltonian is invariant under space inversion (when the space parity is conserved) and time reversal (when time parity is conserved).

Assumption (b) is needed so as to ensure that for given energy the radial Sch. Eq. has only one solution with given l. Conservation of time parity is equivalent to the requirement of a real Hamiltonian ($H^* = H$); hence it follows directly that if ψ is a solution of the Sch. Eq., ψ^* is also a solution.

We should note at this point that the space parity definitely changes in so-called weak interactions, as was conclusively demonstrated in 1957 /92, 93/; recent results also point to nonconservation of time parity /94/. Strong interactions, however, are believed to this day to conserve space and time parity. The following theorems are therefore fully applicable to strong interactions.

We will now consider the general properties of the functions $S_l(k)$ entering the scattering amplitude.*

We have seen that for potentials $U(r)$ which fall off at infinity faster than $1/r$, the Sch. Eq. has two solutions $\chi_{kl}^{(\pm)}$ which behave asymptotically as

$$\chi_{kl}^{(\pm)} \sim e^{\pm i\left(kr - \frac{\pi l}{2}\right)}$$

(the Coulomb potential case is not considered at this stage).

These functions can be formed into a solution which is regular at the origin:**

$$\chi_{kl} = a_l(k)\,\chi_{kl}^{(-)}(r) - b_l(k)\,\chi_{kl}^{(+)}(r), \tag{13.1}$$

where a_l and b_l are some constants dependent only on k. The function clearly vanishes for $r = 0$ if a_l and b_l satisfy the relation

$$\frac{b_l(k)}{a_l(k)} = \lim_{r\to 0} \frac{\chi_{kl}^{(-)}(r)}{\chi_{kl}^{(+)}(r)}. \tag{13.2}$$

From the definition of $S_l(k)$ we have

$$S_l(k) = \frac{b_l(k)}{a_l(k)}. \tag{13.3}$$

Let us consider the general invariance properties of the Sch. Eq. First, since it includes only the square of the wave vector k, the equation is

* A more detailed study of the analytical properties of wave functions and $S_l(k)$ will be found in /95–97/.

** This solution can be normalized using a k-independent condition, say $\lim_{r\to 0} r^{-(l+1)}\chi_l(r) = 1$. In this case, according to Poincaré's theorem /98/, $\chi_l(r)$ is an entire function of k^2.

invariant under a change in the sign of k. Thus if k is replaced by $-k$ in solution (13.1), the new function will also be a solution of the original equation. As the solution is single-valued, however, the two solutions χ_{kl} and χ_{-kl} may differ only by a constant factor. Since the asymptotic expression for the function $\chi_{kl}^{(\pm)}$ gives the relation

$$\chi_{kl}^{(\pm)}(r) = (-1)^l \chi_{-kl}^{(\mp)}(r), \tag{13.4}$$

we find, changing the sign of k in (13.1),

$$\frac{a_l(k)}{b_l(k)} = \frac{b_l(-k)}{a_l(-k)}.$$

Expression (13.3) yields the relation

$$S_l(k) = S_l^{-1}(-k). \tag{13.5}$$

Still another important formula can be derived if we notice that as the Sch. Eq. is real, the complex conjugate of any solution, $\chi_{kl}^{*}(r)$, is also a solution of the Sch. Eq. for real k. As the solution is unique, we again conclude that χ_{kl} and χ_{kl}^{*} may differ only by a constant factor, so that for real k

$$\frac{a_l(k)}{b_l(k)} = \frac{b_l^{*}(k)}{a_l^{*}(k)},$$

i.e.,

$$S_l(k) = (S_l^{-1}(k))^{*}. \tag{13.6}$$

This expression signifies that the two functions $S_l(k)$ and $(S_l^{-1}(k))^{*}$ coincide over the entire real axis in the complex k plane. According to the fundamental theorem of analytical continuation it follows that

$$S_l(k) = (S_l^{*}(k^{*}))^{-1} \tag{13.7}$$

in the entire complex k plane. The previous expressions establish a one-to-one correspondence between the $S_l(k)$ values in the different quadrants of the k plane (Figure 8): if the value of $S_l(k_0)$ at the point k_0 is S_0, we have

$$S_l(k_0^{*}) = \frac{1}{S_0^{*}}, \quad S_l(-k_0^{*}) = S_0^{*}, \quad S_l(-k_0) = \frac{1}{S_0}. \tag{13.8}$$

It is thus sufficient to have the form of $S_l(k)$ in one of the quadrants so as to be able to reconstruct the function $S_l(k)$ for the entire complex plane. The above relations indicate that at points symmetric about the imaginary axis, $S_l(k)$ takes on complex conjugate values. On the imaginary axis, $S_l(k)$ is thus a real function, and the phase $\delta_l(k)$ is a pure imaginary number:

$$\delta_l(\pm i|k|) = -\delta_l^{*}(\pm i|k|). \tag{13.9}$$

For points symmetric about the real axis, we have (13.7). Hence follows the known result: on the real axis $|S_l(k)| = 1$, and the phase $\delta_l(k)$ is real.

Let us now consider the singularities of $S_l(k)$. The regular solution (13.1) can be considered over the entire complex k plane, provided that $\chi_{kl}^{(\pm)}$ are treated as the analytical continuations of the corresponding functions for complex k. In particular, the regular solution will have the same form (13.1) on the imaginary axis. Let the potential $U(r)$ be such that a bound state of the particle exists for some negative energy $-E_0$(or imaginary $k_0 = i|k_0|$). This means that the energy E_0 corresponds to a solution which is regular at the origin and falls off to zero as $e^{ik_0 r} = e^{-|k_0|r}$ at infinity. Since χ_{kl} is the only solution which is regular at the origin, the existence of a bound state implies that the coefficient $a_l(k)$ vanishes

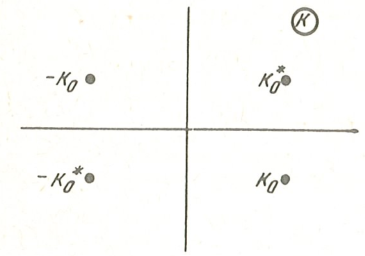

FIGURE 8.

for $k = k_0 = i\sqrt{\frac{2m|E_0|}{\hbar^2}}$; the $\chi_{kl}^{(+)}$ at this point is regular at the origin. Similarly, as for all the k on the imaginary axis in the lower half plane ($k = -i|k|$)

$$\chi_{kl}^{(+)}(r) \to \infty \text{ for } r \to \infty, \; \chi_{kl}^{(-)}(r) \to 0 \text{ for } r \to \infty,$$

the existence of a bound state implies the vanishing of the coefficient $b_l(k)$ at the point $k = -k_0$. This is a reflection of the previously mentioned general invariance property of the Sch. Eq. under sign reversal of k. Returning to (13.3) we come to the conclusion that a bound state corresponds to a pole of the function $S_l(k)$ situated on the imaginary axis in the upper halfplane at the point $k = k_0$.

In accordance with the previously discussed symmetry properties of $S_l(k)$, this pole corresponds to a zero of the function $S_l(k)$ at the point $k = -k_0$ on the imaginary axis in the lower halfplane. Notice also that although a bound state corresponds to a pole, the converse is not always true: not to every pole of $S_l(k)$ on the imaginary axis in the upper halfplane corresponds a bound state. There are so-called "false" or "redundant" poles of $S_l(k)$. We will yet return to this problem at a later stage.

It is readily seen that in the upper halfplane $S_l(k)$ may have poles only on the imaginary axis, so that in the lower halfplane the zeros also lie on the imaginary axis only. Indeed, apart from a common factor, the regular solution (13.1) can be written either as

$$\chi_{kl}(r) = \chi_{kl}^{(-)}(r) - S_l(k)\chi_{kl}^{(+)}(r), \tag{13.10}$$

or as

$$\chi_{kl}(r) = S_l^{-1}(k)\chi_{kl}^{(-)} - \chi_{kl}^{(+)}. \tag{13.10'}$$

If $S_l(k)$ had a pole at a point $k = k_0$ in the upper halfplane not on the imaginary axis, the solution (13.10') would contain only the function χ_{kl}^{+}, which falls off exponentially at infinity:

$$\chi_{kl}(r) \sim -(-i)^l e^{ik_0 r} = -(-i)^l e^{-(-ir \operatorname{Re} k_0 + r \operatorname{Im} k_0)}.$$

But the function $\chi_{kl}(r)$ is by definition regular at the origin, and therefore at the point k_0 this solution would satisfy the two boundary conditions (1.7), i.e., the complex quantity $\frac{\hbar^2 k_0^2}{2m}$ would be an eigenvalue of the Sch. Eq. This is impossible, since any physical potential is real and all the energy eigenvalues are real.

The requirement of a real potential is thus responsible for the concentration of the poles of $S_l(k)$ on the imaginary axis in the upper halfplane. In the lower halfplane, however, no restriction is imposed on the position of the poles, and they may be distributed at random. These conclusions remain in force even if the interaction forces are not potential. The main thing is that the Hamiltonian should be Hermitian.

This theorem can be given an alternative, more formal proof. Consider the time-dependent Sch. Eq. and its conjugate:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + U\psi,$$
$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi^* + U\psi^*.$$

The first equation is multiplied by ψ^*, the second by ψ, and one is subtracted from the other. We get

$$i\hbar\frac{\partial}{\partial t}|\psi|^2 = -\frac{\hbar^2}{2m}\nabla(\psi^*\nabla\psi - \psi\nabla\psi^*).$$

Integration of this equation over an arbitrary volume V enclosed within a surface S gives the law of particle number conservation:

$$\frac{\partial}{\partial t}\int_V |\psi|^2 dr = \oint_S dS\frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*). \qquad (13.11)$$

Let now $S(k)$ have a pole at some point $k_0 = k_1 + ik_2$. The wave function at this point has the form

$$\psi = \frac{1}{r}\chi(r)e^{-\frac{iEt}{\hbar}} \sim \frac{1}{r}e^{i(k_1+ik_2)r - \frac{i\hbar}{2m}(k_1^2-k_2^2+2ik_1k_2)t}.$$

Inserting this expression in (13.11), we choose the volume V as the inside of a sphere of radius $r = R$, where R is sufficiently large so that on the surface of the sphere we may use the asymptotic expression for the wave function. Elementary manipulations give

$$k_1k_2\int_0^R |\chi(r)|^2 dr = -\frac{k_1}{2R^2}e^{-2Rk_2}.$$

Since there is a minus sign in the right-hand side, this equality is satisfied only if

(a) $k_1 = 0$, i.e., the pole of $S(k)$ lies on the imaginary axis,

(b) $k_1 \neq 0$, $k_2 < 0$, i.e., the pole of $S(k)$ lies in the lower halfplane.

This completes the proof of the theorem.

The only constraint on the position of the poles in the lower halfplane is that they should occur in pairs symmetrically about the imaginary

axis.* The zeros of $S_l(k)$ in the lower halfplane, however, may lie only along the imaginary axis. This follows from (13.5).

Poles in the upper halfplane correspond as a rule to bound states of particles in the field $U(r)$. For poles in the lower halfplane the regular (at the origin) wave function has the asymptotic form

$$\left.\begin{aligned} \chi_{kl}(r) &\sim -(-i)^l e^{ikr} = -(-i)^l e^{ir\,\mathrm{Re}\,k + r\,|\mathrm{Im}\,k|}, \\ \chi_{kl}(r) &\to \infty \text{ for } r \to \infty, \end{aligned}\right\} \qquad (13.12)$$

i.e., it diverges at infinity.

This wave function thus does not satisfy the boundary condition at infinity and would seem to be physically meaningless. This is not quite so, however. In Chapter 5 we will see that to every pole of $S_l(k)$ in the lower halfplane corresponds a so-called quasistationary state of the particle in the field $U(r)$, i.e., a state which, once formed, will have a finite lifetime τ.

Let us sum up what we have learned on the topography of the function $S_l(k)$ in the complex plane. This function is analytical in the entire complex k plane, with the possible exception of isolated singularities and cuts. In the upper halfplane it may have poles on the imaginary axis only. Some of these poles correspond to bound states, other are "false" poles. In the next section we will give a prescription for identifying the "false" poles. $S_l(k)$ may have zeros in the upper halfplane and corresponding poles in the lower halfplane. On the imaginary axis $S_l(k)$ is real and on the real axis its modulus is equal to unity. If the wave vector k is replaced by energy, we should remember that the k plane is mapped onto a two-sheet E plane. Bound states correspond to poles on the left semiaxis in the upper E plane. The poles on the lower sheet of the E plane correspond to quasistationary states.

In what follows we will require the symmetry properties of scattering phases. On the real axis the phase δ is real. By (13.5) we see that for real k

$$\delta_l(k) = -\delta_l(-k). \qquad (13.13)$$

Wave functions normalized to $\delta(k - k')$ have the asymptotic expression

$$\chi_{kl} \sim \sqrt{\frac{2}{\pi}}\sin\left(kr + \delta(k) - \frac{\pi l}{2}\right).$$

Using this expression, we can readily verify that as the sign of k changes, the wave functions behave in the following way:

$$\chi_{k,l}(r) = (-1)^{l+1}\chi_{-k,l}(r). \qquad (13.14)$$

We have mentioned in the preceding that $S_l(k)$ is an analytic function in the complex k plane. This holds true for any potential and is a consequence

* For potentials vanishing for $r > R$ there is an infinity of such poles /99—101/; in this case the distribution of the distant poles is completely determined by the behavior of the potential for $r \to R$. The poles in case of a rectangular box were treated in detail in /102/.

of the principle of physical causality.* In other words, the cause must precede the effect. This is an inevitable prerequisite of any physical theory, and it is found to have very far-reaching consequences. We will now try to sketch a rough outline of the formal results emerging from the causality principle.

We write the expression for the wave function for given energy E at some distance $r = a$ outside the effective range of the potential:

$$(e^{-ika} - S(E)\, e^{ika})\, e^{-\frac{iEt}{\hbar}}.$$

The first term corresponds to the incoming wave and the second to the outgoing wave. A spatially localized wave packet is given by

$$\int_0^\infty dE' \left(f(E')\, e^{-ik'a} - g(E')\, e^{ik'a}\right) e^{-\frac{iE't}{\hbar}},\quad g(E') = S(E')\, f(E'). \tag{13.15}$$

The wave packet describing the incoming waves is clearly

$$\Phi_{\text{in}}(a, t) = \int_0^\infty dE' f(E')\, e^{-ik'a - \frac{iE't}{\hbar}},$$

and the wave packet of the outgoing waves is

$$\Phi_{\text{out}}(a, t) = \int_0^\infty dE' g(E')\, e^{ik'a - \frac{iE't}{\hbar}}.$$

Since the system is linear and the amplitude of the divergent outgoing waves is fully determined by the incident wave, we have the following relation between the two amplitudes:

$$\Phi_{\text{out}}(a, t) = \int_{-\infty}^{\infty} H(t - t')\, \Phi_{\text{in}}(a, t')\, dt', \tag{13.16}$$

where H is some transformation kernel.

It is here that the causality principle enters the discussion: the amplitude of the outgoing wave at the time t can depend on $\Phi_{\text{in}}(t')$ only if $t > t'$. We must therefore have

$$H(t - t') = 0 \quad \text{for} \quad t' > t. \tag{13.17}$$

Introducing the Fourier component $h(\omega)$ of the operator H,

$$H(\tau) = \int_{-\infty}^{\infty} d\omega\, e^{-i\omega\tau} h(\omega), \tag{13.18}$$

we easily find from (13.15)—(13.18) that

$$h(E) = \frac{1}{2\pi} e^{2ika} S(E). \tag{13.19}$$

* This idea was first advanced in /103/, but the original proof is not fully rigorous. The rigorous proof first given by Van Kampen /104/ requires knowledge of comparatively fine theorems of the theory of analytic functions.

Inverting (13.18), we get

$$e^{2ika} S(E) = +\int_{-\infty}^{\infty} e^{iE\tau} H(\tau)\, d\tau.$$

In the general case, this expression sheds no light on the properties of $S(E)$. By the causality principle, however (see (13.17)), we know that $H(\tau) = 0$ for $\tau < 0$. The integration should therefore start from zero:

$$e^{2ika} S(E) = +\int_0^{\infty} e^{iE\tau} H(\tau)\, d\tau. \tag{13.20}$$

In this case the function in the right-hand side is clearly analytical in the upper E halfplane, where $e^{iE\tau}$ decays exponentially. In the k plane this corresponds to the first quadrant. Thus, using the symmetry properties of $S(k)$, we find that $S(k)$ is analytic in all the quadrants. The exponential factor e^{2ika} in (13.20) accounts for the phase lead of the wave reflected from the spherical surface $r = a$ relative to the wave passing through the scattering center /105/ (the corresponding path length difference is $2a$).

For a plane wave scattered at a finite angle θ we should choose the shortest path (corresponding to maximum phase lead) through the scattering sphere which reaches the observer at an angle θ (Figure 9). This path length is less by $2a\sin\frac{\theta}{2}$ than the length of the path through the scattering center. Therefore, in the upper E halfplane, it is the function $e^{2ika\sin\frac{\theta}{2}} f(E, \theta)$ that is analytic, and not the scattering amplitude $f(E, \theta)$. Hence it is clear that the simplest analytical properties are characteristic of $f(E, 0)$ (it is analytic in the upper E halfplane).

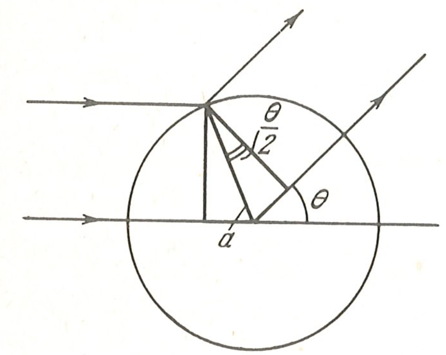

FIGURE 9.

The causality principle can be applied to derive the analyticity properties of the scattering amplitude from momentum transfer /106/. Note that the validity of our assertions on analyticity is independent of the particular form of the potential for $r < a$. Moreover, even the assumption that the wave function inside the interaction range ($r < a$) satisfies the Sch. Eq. is unnecessary. In other words, the analyticity of $S(E)$ in the upper E halfplane is a direct consequence of the causality principle alone. This problem is discussed in /107, 108/.

§ 14. "FALSE" POLES

We have already mentioned that in the upper halfplane $S_l(k)$ may have so-called "false" poles* on the imaginary axis, which do not correspond to

* The existence of these poles was first pointed out by Ma /109/ [who called them "redundant"].