MATSCIENCE REPORT 20

LECTURES ON

AN INTRODUCTION TO DISPERSION RELATION TECHNIQUES

BY

PROF. P. ROMAN

Visiting professor, MATSCIENCE

Notes prepared by

G. JAGANNATHAN and P. SRIDHAR RAO

THE INSTITUTE OF MATHEMATICAL SCIENCES, MADRAS-4, INDIA.

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AN INTRODUCTION TO DISPERSION RELATION TECHNIQUES

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Professor Paul Roman*
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MATSCIENCE, Madras.

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Notes by
G. Jagannathan and P. Sridhar Rao

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* Professor of Physics, Boston University, Mass., U.S.A.

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CONTENTS

AN INTRODUCTION TO DISPERSION RELATION TECHNIQUES

Chapter I.

INTRODUCTION:

The recent developments in the theory of elementary particles are characterised by a desire to probe deep into the fundamental. In the last decade it has been realised with increasing seriousness that in the conventional theory of elementary particles which is based essentially on quantum field theory the presently available methods of collision theory are inadequate to unravel many relevant features of the elementary interactions. These difficulties are in part due to the following reasons:

(1) In quantum field theory the interaction cannot be characterised by a localised potential.

(2) There are no reliable approximation methods to treat strong interactions.

Therefore the need was felt to lean heavily on experimental data such as cross-sections, bound states and resonances. Attempts are being made to deduce basic features of the interaction such as strength and range from general structural assumptions.

It is even hoped that such structural type of investigations may lead to a discipline which may be so complete and consistent as to replace the conventional Hamiltonian or Schrodinger equation approach or at least, the structural consideration may give rise to more powerful approximation methods.

These new trends are now commonly referred to as dispersion relation techniques. The scope of this mathematical tool

is manifest only in the relativistic quantum theory of elementary particles, and there is little need for them in the framework of non-relativistic potential scattering. Nevertheless an application of these methods to elementary point-quantum-mechanics elucidates the basic features of this new approach.

The idea behind the dispersion relation techniques is as follows. We consider a physically significant function such as the scattering amplitude. This is in general a function of the real variables k (momentum) and ϑ (the scattering angle) The first step consists in analytically continuing the function to complex values of its argument. Then we proceed to determine its analytic behaviour from the general structure of the underlying theory and the singularities are given a physical interpretation. We invoke Cauchy's theorem to express these analytic properties in a compact form. The resulting mathematical expression is called a dispersion relation.

The Kramers-Kronig Dispersion Relation:

The Kramers-Kronig relation is the fore-runner of the modern dispersion relations. From the classical theory of dispersion of light, the following relation between the real and imaginary parts of the complex index of refraction can be obtained

$$n(\omega) = 1 + \frac{c}{\pi} P \int_0^\infty \frac{\alpha(\omega')}{\omega'^2 - \omega^2} d\omega' \qquad (1)$$

where $n(\omega)$ = Index of refraction for light of frequency ω and $\alpha(\omega)$ = Absorption coefficient of the medium for ω and P denotes principal value.

Let us define $N(\omega)$, the complex refractive index, as follows:

$$\text{Re}\ N(\omega) = n(\omega) \tag{2a}$$

$$\text{Im}\ N(\omega) = \frac{c}{2\omega}\,\alpha(\omega) \tag{2b}$$

Here in (2b) $c/2\omega$ is introduced to make Im $N(\omega)$ dimensionless. To extend $N(\omega)$ to negative frequency ranges, we define*

$$N(-\omega) = N^{*}(\omega) \tag{3}$$

Using the above definitions equation (1) can be written as

$$\text{Re}\left[N(\omega)-1\right] = \frac{2}{\pi} P\int_{0}^{\infty} \frac{\omega' \,\text{Im}\left[N(\omega')-1\right]}{\omega'^{2}-\omega^{2}}\, d\omega' \tag{4a}$$

or alternatively

$$\text{Re}\left[N(\omega)-1\right] = \frac{1}{\pi} P\int_{-\infty}^{\infty} \frac{\text{Im}\left[N(\omega')-1\right]}{\omega'-\omega}\, d\omega' \tag{4b}$$

This is the real part of the equation

$$N(\omega)-1 = \frac{1}{\pi i} P\int_{-\infty}^{\infty} \frac{N(\omega')-1}{\omega'-\omega}\, d\omega' \tag{5}$$

or

$$N(\omega)-1 = \lim_{\epsilon \to +0} \frac{1}{\pi i}\int_{-\infty}^{\infty} \frac{N(\omega')-1}{\omega'-\omega-i\epsilon}\, d\omega' \tag{6}$$

Let us suppose that $N(\omega)$ can be extended to complex values of ω also. Let us further assume

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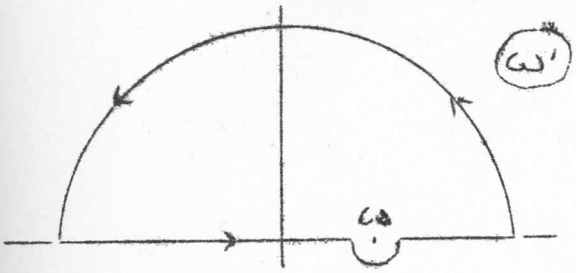
* The following notation will be used hereafter:
The complex conjugate of A is written A^{*}.
The Hermitean conjugate of A is written A^{*}.

(i) that $N(\omega) - 1$ has no singularities in the upper half plane,

and (ii) that $N(\omega) - 1 \to 0$ as $|\omega| \to \infty$, in the upper half-plane. This defines the asymptotic behaviour of $N(\omega) - 1$ and this condition plays a crucial role in determining the structure of dispersion relations.

Using Cauchy's integral formula, we have



$$N(\omega) - 1 = P \frac{1}{\pi i} \int_{-\infty}^{\infty} \frac{N(\omega') - 1}{\omega' - \omega} d\omega' \qquad (7)$$

The crucial point is that condition (i) can be justified by appealing to the condition that signals can not be propagated with a velocity greater than that of light. Thus the principle of causality necessitates certain analyticity properties, and results in the dispersion relation (7).

Let us rewrite the above relation in terms of electromagnetic scattering amplitude. To this end we invoke the relation first given by Lorentz between scattering amplitude and refractive index,

$$N(\omega) = 1 + \frac{2\pi c^2}{\omega^2} p f(\omega, 0) \qquad (8)$$

where p = no of scattering centers/unit volume

and f = scattering amplitude as a function of ω for the scattering angle ϑ (here equal to zero).

We substitute (8) in (4a) and get

$$\mathrm{Re}\, f(\omega,0) = \frac{2\omega^2}{\pi} P\int_0^\infty \frac{\mathrm{Im}\, f(\omega',0)}{\omega'(\omega'^2-\omega^2)}\, d\omega' \qquad (9)$$

The physical significance of the above equation may be seen clearly by making use of the optical theorem:

$$\sigma(\omega) = \frac{4\pi c}{\omega}\ \mathrm{Im}\ f(\omega,0) \qquad (10)$$

where $\sigma(\omega)$ = the total scattering cross-section. Hence (9) becomes:

$$\mathrm{Re}\ f(\omega,0) = \frac{\omega^2}{2\pi^2 c}\ P\int_0^\infty \frac{\sigma(\omega')}{\omega'^2-\omega^2}\, d\omega' \qquad (11)$$

Now, experimental measurements yield only $|f(\omega,0)|^2$. The importance of equation (11) consists in yielding $f(\omega,0)$ itself in terms of $\sigma(\omega)$, which is experimentally measurable. However, this is true only of forward scattering; for nonforward scattering the expression is more complicated.

Equation (9) or (11) is valid only for the bound electrons in the atoms of the scatterer. This can be seen by allowing $\omega \to 0$, in which case the scattering amplitude also $\to 0$. Hence

$$f(0,0) = 0$$

This is physically true since bound electrons do not respond to 'zero frequency' field. However free electrons do respond to such a static electromagnetic field and so in their case $f(0,0) \neq 0$.

The anomaly arose because for free electrons the asymptotic condition is actually $f(\omega) \to \infty$ as $\omega \to \infty$. This

difficulty is frequently met with in dispersion relations.

The correct relation is obtained by making a 'subtraction' as follows: From equation (11)

$$\text{Re } f(\infty, 0) = -\frac{1}{2\pi^2 c} P \int_0^\infty \sigma(\omega')\, d\omega' \qquad (12)$$

Subtracting (12) from (11),

$$\text{Re } f(\omega, 0) - \text{Re } f(\infty, 0) = \frac{1}{2\pi^2 c} P \int_0^\infty \frac{\omega'^2 \sigma(\omega')}{\omega'^2 - \omega^2}\, d\omega' \qquad (13)$$

This is called the subtracted dispersion relation which is valid for free electrons as well. As $\omega \to \infty$ both sides of the equation $\to 0$. (Though the validity of the procedure of subtracting ∞ from both sides appears doubtful, it can be justified mathematically.)

The unmeasurable constant $f(\infty, 0)$ in equation (13) can be removed by first putting $\omega = 0$ in the same equation:

$$\text{Re } f(0,0) - \text{Re } f(\infty, 0) = \frac{1}{2\pi^2 c} P \int_0^\infty \sigma(\omega')\, d\omega' \qquad (14)$$

(13) and (14) gives, the Kramers-Kronig dispersion relation:

$$\text{Re } f(\omega, 0) - \text{Re } f(0, 0) = \frac{\omega^2}{2\pi^2 c} P \int_0^\infty \frac{\sigma(\omega')}{\omega'^2 - \omega^2}\, d\omega' \qquad (15)$$

The constant Re f (0, 0) can be calculated on the basis of classical electromagnetic theory.

Chapter II.

MATHEMATICAL TECHNIQUES

Here a general procedure is given by which dispersion relations can be deduced once the analytic behaviour of a function is known.

(i) A function $f(x)$, such as the scattering amplitude, may be analytically continued to complex values of the argument. If the following conditions hold, namely

(a) $f(z)$ is regular in the upper half-plane, i.e. for

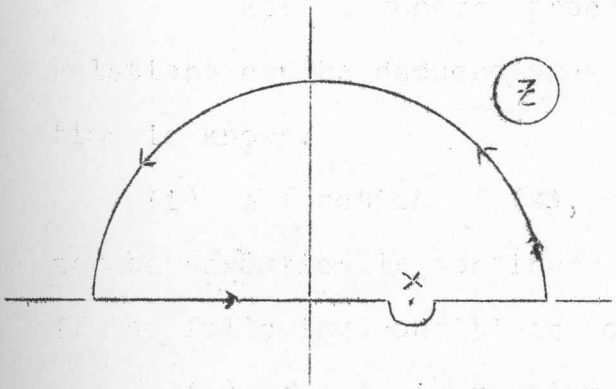
$$\text{Im } z > 0$$

and (b) $f(z) \to 0$ as $|z| \to \infty$

then Cauchy's integral formula is applicable,

$$f(z) = \frac{1}{2\pi i} \oint_C \frac{f(z')}{z' - z} dz' \qquad (16)$$

where z is inside the contour. If z is outside the contour the integral vanishes. If z is on the contour, the contour has to be suitably indented.



Let C be a semi-circle of infinite radius and the real axis. The contribution along the semi-circle vanishes.

If $z = x$, then

$$f(x) = \lim_{y \to +0} f(x + iy)$$

$$= \lim \frac{1}{\pi i} \int^{\infty} \frac{f(x')}{\quad} dx'$$

But $$P\int_{-\infty}^{\infty} \frac{f(x')}{x'-x}\,dx' = \lim_{y\to+0}\int_{-\infty}^{\infty} \frac{f(x')}{x'-(x+iy)}\,dx'$$

or $$f(x) = \frac{1}{2\pi i} P\int_{-\infty}^{\infty} \frac{f(x')}{x'-x}\,dx' \qquad (17)$$

Taking real and imaginary parts of equation (17),

$$\text{Re } f(x) = \frac{P}{2\pi}\int_{-\infty}^{\infty} \frac{\text{Im } f(x')}{x'-x}\,dx' \qquad (18a)$$

$$\text{Im } f(x) = -\frac{P}{2\pi}\int_{-\infty}^{\infty} \frac{\text{Re } f(x')}{x'-x}\,dx' \qquad (18b)$$

These are called unsubtracted dispersion relations, and relate the real and imaginary parts of $f(x)$.

In mathematical literature, the functional

$$\mathcal{H}[u] = \frac{P}{\pi}\int_{-\infty}^{\infty} \frac{u(x')}{x'-x}\,dx'$$

is called the Hilbert transform of the function $u(x)$. So equations (18a) and (18b) merely imply that the real and imaginary parts of $f(x)$ are connected by a Hilbert transformation.

The function $f(x)$ is originally known only for $x > 0$ but may be analytically continued to the negative values of the argument by appealing to the so called crossing symmetry relation

$$f(-x) = f^*(x) \qquad (19)$$

which, in the case of potential scattering, follows from the hermiticity of the Hamiltonian. Then, because

$$\int_{-\infty}^{0} \frac{\mathrm{Im}\ f(x')}{x' - x}\, dx' = \int_{0}^{\infty} \frac{\mathrm{Im}\ f(x')}{x' + x}\, dx'$$

the dispersion relation (18a) can be thrown in the form

$$\mathrm{Re}\ f(x) = \frac{1}{\pi} P \int_{0}^{\infty} \frac{x'\ \mathrm{Im}\ f(x')}{x'^2 - x^2}\, dx' \qquad (20)$$

This form of the dispersion relation is the one most frequently employed.

(ii) Suppose there are N finite isolated poles in the upper half plane at z_i ($i = 1, 2, \ldots N$). Let Γ_i be the residue of $f(z)$ at $z = z_i$. Then

$$f(z) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{f(x')}{x' - z}\, dx' + \sum_{i=1}^{N} \frac{\Gamma_i}{z - z_i} \qquad (21)$$

If $z = x$, a point on the real axis

$$\mathrm{Re}\ f(x) = \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{Im}\ f(x')}{x' - x}\, dx' + \mathrm{Re} \sum_{i}^{N} \frac{\Gamma_i}{x - z_i} \qquad (22)$$

(iii) Suppose the asymptotic condition is now

$f(z) \to C$, a constant, as $|z| \to \infty$

(a) Let there be no singularities in the upper half plane.

The integral along the infinite semi-circle does not vanish. But Cauchy's theorem may be applied to the function

$$f(z) - f(\infty)$$

since this does vanish at $|z| \to \infty$. The dispersion relation

becomes

$$f(z) - f(\infty) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{f(x') - f(\infty)}{x' - z} \, dx' \tag{23}$$

If $z = x$, a point on the real axis, then the second term does not contribute since by definition

$$P \int_{-\infty}^{\infty} \frac{1}{x' - x} \, dx' = 0 \tag{24}$$

Hence, taking real parts,

$$\mathrm{Re}\, f(x) - \mathrm{Re}\, f(\infty) = \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{Im}\, f(x')}{x' - x} \, dx' \tag{25}$$

To remove $f(\infty)$ which is not measurable, we use the known value of $f(x)$ at some convenient $x = x_0$. Substituting $x = x_0$ in equation (25) and subtracting the resulting equation from equation (25) itself:

$$\mathrm{Re}\, f(x) - \mathrm{Re}\, f(x_0) = (x - x_0) \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{Im}\, f(x')}{(x' - x)(x' - x_0)} \, dx' \tag{26}$$

(b) Let there be N poles in the upper half-plane. The modified formula is then

$$f(x) - f(x_0) = \frac{(x - x_0)}{\pi i} P \int_{-\infty}^{\infty} \frac{f(x') \, dx'}{(x' - x)(x' - x_0)} + \sum_{i=1}^{N} \frac{\Gamma_i (x - x_0)}{(x - z_i)(x_0 - z_i)} \tag{27}$$

(iv) (a) Suppose $f(z) \to \sum_{j=0}^{n} a_j z_j$ for $|z| \to \infty$. Further assume that $f(z)$ is regular in the upper-half plane. Then it can be shown that

$$\mathrm{Re}\, f(x) - \sum_{j=0}^{n} \frac{(x - x_0)^j}{j!} \mathrm{Re}\, g_j = \frac{(x - x_0)^{n+1}}{\pi} P \int_{-\infty}^{\infty} \frac{\mathrm{Im}\, f(x') \, dx'}{(x' - x)(x' - x_0)} \tag{28}$$

where

$$q_j = \left(\frac{d^j f}{d x^j} \right)_{x = x_o}$$

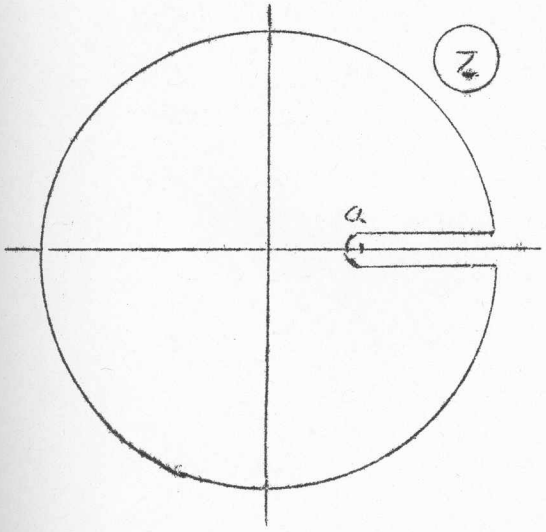
So we need to know only the function and its n derivatives at <u>one</u> point x_o .

(b) In case f (z) has finite number of poles we have to add the corresponding pole terms.

(v) Suppose there is a branch point on the real axis. Assume that the only singularity is the branch point at $x = a$ and the function f(z) is regular everywhere else. Further

$$f(z) \to 0 \quad \text{as} \quad |z| \to \infty .$$

For convenience let the branch cut be taken along the real axis from a to ∞ . The contribution to the integral comes



only from the integration along the cut:

$$f(z) = \frac{1}{\pi} \int_a^\infty \frac{\rho(x')}{x' - z} \, dx' \qquad (29)$$

where

$$\rho(x') = \lim_{\epsilon \to +0} \frac{1}{2i} \left[f(x' + i\epsilon) - f(x' - i\epsilon) \right]$$

Suppose f (x) is real for $x \leq a$. Using Schwartz reflection principle

$$f(z^*) = f^*(z) \qquad (30)$$

we arrive at the following results

$$\rho(x') = I_m\, f(x')$$

and

$$f(x) = \frac{1}{\pi}\int_a^\infty \frac{I_m\, f(x')}{x'-x}\, dx'$$

Then

$$R_e\, f(x) = \frac{1}{\pi}\int_a^\infty \frac{I_m\, f(x')}{x'-x}\, dx' \qquad (31)$$

Equation (31) is similar to Hilbert transform with the following differences:

(1) The lower limit of (31) is a and not 0.

(2) Here we are not concerned with the principal value.

and (3) Equation (31) is true only for $x \leq a$.

(vi) If all the simplifying assumptions about $f(z)$ are relaxed, we get

$$f(z) - \sum_{j=0}^{n} \frac{(z-z_0)^j}{j!}\, q_j = \sum_{i=1}^{N} \frac{\Gamma_i (z-z_0)^{n+1}}{(z-z_i)(z_0-z_i)^{n+1}} + \frac{(z-z_0)^{n+1}}{\pi}\int_a^\infty \frac{\rho(x')\, dx'}{(x'-z)(x'-z_0)^{n+1}} \qquad (32)$$

where $f(z)$ has the following properties:

(i) $f(z)$ has poles at $z = z_i$ $(i = 1, 2, \ldots\ldots N)$ in the upper half plane.

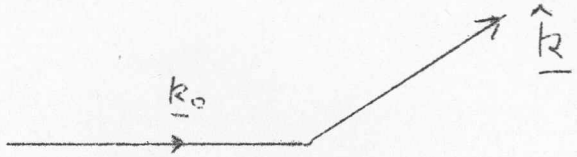
(2) $f(z)$ has a branch cut from $x = a$ to $x = \infty$.

(3) $f(z) \to \sum_{j=0}^{n} a_j\, z^j$ as $|z| \to \infty$.

Chapter III.

DISPERSION RELATION FOR POTENTIAL SCATTERING

We will now consider the scattering of spinless particle by a central potential. Let the incoming particles have a momentum $\underline{k}_0$.



The Schrodinger equation describing the process is

$$\left[\nabla^2 + k^2 - U(r)\right] \psi_k^+(\underline{r}) = 0 \qquad (33)$$

where $U(r) = \frac{2m}{\hbar^2} V(r)$ [A central potential is assumed] and

$$E = \hbar^2 k^2 / 2m$$

The subscript k in the wave function distinguishes solutions for different k . The superscript + is inserted to denote the outgoing solution. The asymptotic behaviour of ψ_k^+ is

$$\psi_k^+ \approx e^{i\underline{k}_0 \cdot \underline{r}} + f(k, \vartheta) \frac{e^{ikr}}{r} \qquad (34)$$

For a central potential

(i) f is independent of the azimuth

and (ii) $|\underline{k}_0| = |\hat{\underline{k}}| = k$

The wave function ψ_k^+ can be thought of as made up of two parts.

$$\psi_k^+ = \varphi + \Phi \qquad (35)$$

where φ represents the free wave and Φ the scattered wave.

φ is a solution of the unperturbed Schrodinger equation

$$\left(\nabla^2 + k^2\right) \varphi = 0 \tag{36}$$

From (34) we can write

$$\varphi = e^{i \underline{k}_0 \cdot \underline{r}} \tag{37}$$

Substituting (35) in (33), we have

$$\left[\nabla^2 + k^2 - U(r)\right] \Phi(r) = U(\underline{r})\, \varphi(\underline{r}) \tag{38}$$

This is the differential equation satisfied by the scattered wave. The solution is obtained using the Green's function $g(\underline{r}, \underline{r}'; k)$ given by

$$\left[\nabla^2 + k^2 - U(r)\right] g(\underline{r}, \underline{r}'; k) = \delta(\underline{r} - \underline{r}') \tag{39}$$

From equations (38) and (39) we derive the source representation for Φ :

$$\Phi(\underline{r}) = \int g(\underline{r}, \underline{r}'; k)\, U(r')\, \varphi(\underline{r}')\, d^3\underline{r}'$$

$$= \int g(\underline{r}, \underline{r}'; k)\, U(r')\, e^{i \underline{k}_0 \cdot \underline{r}'}\, d^3\underline{r}' \tag{40}$$

Now g can be expressed in terms of another Green's function $G^+(\underline{r}, \underline{r}', k)$ given by

$$\left(\nabla^2 + k^2\right) G^+(\underline{r}, \underline{r}'; k) = -\delta(\underline{r} - \underline{r}') \tag{41}$$

whose solution is

$$G^+(\underline{r}, \underline{r}'; k) = \frac{1}{4\pi} \frac{e^{ik|\underline{r} - \underline{r}'|}}{|\underline{r} - \underline{r}'|} \tag{42}$$

If equation (39) is rewritten as

$$\left(\nabla^2 + k^2\right) g\left(\underline{r}, \underline{r}'; k\right) = \delta\left(\underline{r} - \underline{r}'\right) + U(r)\, g\left(\underline{r}, \underline{r}' k\right) \tag{43}$$

then equations (41) and (43) lead directly to the integral equation:

$$-g(\underline{r}, \underline{r}'; k) = G(\underline{r}, \underline{r}'; k) + \int G(\underline{r}, \underline{r}'', k)\, U(r'') \, g(\underline{r}'', \underline{r}'; k)\, d^3 r'' \tag{44}$$

This can be solved under given boundary conditions, so that g is known explicitly in terms of G which is given by equation (42). Thus ψ_k^+ is given by

$$\psi_k^+(\underline{r}) = e^{i \underline{k}_0 \cdot \underline{r}} + \int g(\underline{r}, \underline{r}'; k)\, U(r')\, e^{i \underline{k}_0 \cdot \underline{r}'}\, d^3 \underline{r}' \tag{45}$$

Now equation (33) can be written

$$\left(\nabla^2 + k^2\right) \psi_k^+(\underline{r}) = U(r)\, \psi_k^+(\underline{r})$$

which becomes, using equation (35)

$$\left(\nabla^2 + k^2\right) \Phi(\underline{r}) = U(r)\, \psi_k^+(\underline{r})$$

This equation, taken with (41) and (42), yields

$$\Phi(\underline{r}) = -\frac{1}{4\pi} \int \frac{e^{i k |\underline{r} - \underline{r}'|}}{|\underline{r} - \underline{r}'|}\, U(\underline{r}')\, \psi_k^+(r')\, d^3 \underline{r}' \tag{46}$$

For large r, this becomes

$$\Phi(\underline{r}) \approx -\frac{1}{4\pi} \frac{e^{i k r}}{r} \int e^{-i \hat{\underline{k}} \cdot \underline{r}'}\, U(r')\, \psi_k^+(\underline{r}')\, d^3 \underline{r}' \tag{46a}$$

Comparing with equation (34), the expression for scattering amplitude $f(k, \vartheta)$ is seen to be

$$f(k,\vartheta) = -\frac{1}{4\pi} \int e^{-i\hat{\underline{k}}\cdot\underline{r}} U(r') \psi_k^{+}(\underline{r}') \, d^3\underline{r}' \tag{47}$$

This integral contains the exact solution $\psi_k^{+}(r')$ of the Schrodinger equation. By direct substitution of equation (45) in (47) we have:

$$f(k,\vartheta) = -\frac{1}{4\pi} \int e^{-i(\hat{\underline{k}}-\underline{k}_0)\cdot\underline{r}} U(r) \, d^3\underline{r}$$

$$-\frac{1}{4\pi} \iint e^{-i\hat{\underline{k}}\cdot\underline{r}} e^{i\underline{k}_0\cdot\underline{r}'} U(r) g(\underline{r},\underline{r}';k) U(r') \, d^3\underline{r} \, d^3\underline{r}' \tag{48}$$

It is convenient to introduce the momentum transfer $\underline{\Delta}$ in the place of ϑ. $\underline{\Delta}$ is defined by

$$\underline{\Delta} = \hat{\underline{k}} - \underline{k}_0 \tag{49}$$

From elementary considerations, it can be proved

$$|\underline{\Delta}| \equiv \Delta = 2k \sin\frac{\vartheta}{2} \tag{50}$$

Also it can be proved using equation (40) and the symmetry of G^+ with respect to $\underline{r}$ and $\underline{r}'$ that

$$g(\underline{r},\underline{r}';k) = g(\underline{r}',\underline{r};k) = g^{*}(\underline{r},\underline{r}';-k) \tag{51}$$

Since our ultimate aim is to extend $f(k, \vartheta)$ to the complex plane, we first extend g to complex values of k with the reservation that $U(r)$ is real; i.e. we are considering elastic scattering. Now we quote a theorem which is helpful in studying the analytic properties of g..

Theorem:

If Ω is any hermitian differential operator, and if g is the solution of the differential equation,

$$(\Omega + z^2) g = \delta(\underline{r} - \underline{r}') \quad , \quad \mathrm{Im}\, z > 0 \tag{52}$$

then g possesses the bilinear expansion

$$g(\underline{r}, \underline{r}'; k) = \sum_{i=1}^{N} \frac{\varphi_i(\underline{r})\, \varphi_i^*(\underline{r}')}{z^2 - z_i^2} + \int \frac{\psi_{k'}(\underline{r})\, \psi_{k'}(\underline{r}')}{z^2 - k'^2}\, d^3k' \tag{53}$$

where φ_i is the eigenfunction corresponding to a discrete eigenvalue z_i^2 of Ω:

$$\Omega \varphi_i = z_i^2 \varphi_i \quad , \quad i = 1, 2, \ldots N. \tag{54}$$

and ψ_k's are eigenfunctions of the continuum part of the spectrum,

$$\Omega \psi_{k'} = k'^2 \psi_{k'} \tag{55}$$

We note the following points:

(1) z_i^2 are real and < 0

(2) $z^2 = z_i^2$ are the poles of g

$z = + i\, |z_i|$; positive sign is chosen because $\mathrm{Im}\, z > 0$

$= i \sqrt{|\epsilon_i|}$ (later ϵ_i are interpreted as the energies of the bound states).

(3) The second term of the expansion of g has a cut on the positive real axis. This follows from the following general considerations.

If $R(x) = \int_a^\infty \frac{F(y)}{x-y}\, dy$

then R has a branch-cut from $x = a$ to $x = \infty$. By setting $x = x + i\eta$ and $x = x - i\eta$ and taking the limit $\eta \to \pm 0$ we can compute the discontinuity of R for $x > a$, if any.

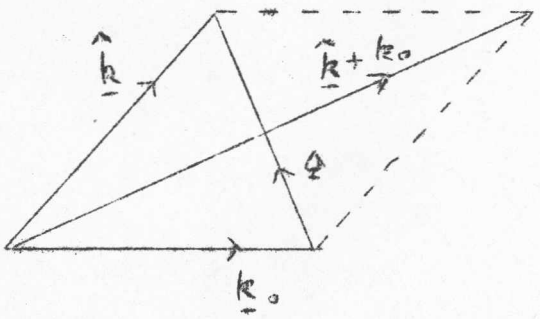
Let us define an auxiliary vector $\underline{q}$ by

$$\underline{q} = \tfrac{1}{2}\left(\hat{\underline{k}} + \underline{k}_0\right) \tag{56}$$

$$q = \left(k^2 - \frac{\Delta^2}{4}\right)^{1/2} \tag{57}$$

$\underline{q} = q\,\underline{n}$; $\underline{n}$ is the unit vector pointing in the direction of $(\hat{\underline{k}} + \underline{k}_0)$.

Note that $\underline{q} \cdot \underline{\Delta} = 0$ because $\underline{k} - \underline{k}_0$ is $\perp$ to $\hat{\underline{k}} + \underline{k}_0$



It is easily proved using the definitions of $\underline{\Delta}$ and $\underline{q}$ that

$$\hat{\underline{k}} \cdot \underline{t} - \underline{k}_0 \cdot \underline{t}' = \tfrac{1}{2}\,\underline{\Delta} \cdot (\underline{t} + \underline{t}') + q\,\underline{n}\,(t - t')$$

Then equation (48) can be written in terms of Δ and k as

$$f(k,\Delta) = f_B(\Delta) - \frac{1}{4\pi}\iint \exp\left[-\frac{i}{2}\underline{\Delta}\cdot(\underline{r}+\underline{r}')\right]\exp\left[i\left(k^2-\frac{\Delta^2}{4}\right)^{1/2}\underline{n}\cdot(\underline{r}'-\underline{r})\right] U(r)\, g(\underline{r},\underline{r}';k)\, U(r')\, d^3r'\, d^3r \tag{58}$$

where $f_B(\Delta) = -\frac{1}{4\pi}\int e^{-i\underline{\Delta}\cdot\underline{r}}\, U(r)\, d^3r$ is the first Born approximation. This is actually the Fourier transform of U (r). It is to be noted that f_B depends only on Δ.

We investigate the properties of the scattering amplitude for <u>fixed</u> momentum transfer Δ and arbitrary k .

To start with, we extend f (k, Δ) to real negative values of k . By invoking the hermiticity condition satisfied by the Green's function (equation 51), we obtain the crossing symmetry relation

$$f(-k,\Delta) = f^*(k,\Delta) \tag{59}$$

for real k .

But by equation (50),

$$\Delta = 2k \sin\frac{\vartheta}{2}$$

and hence for real values of ϑ,

$$k \geq \frac{1}{2}\Delta \tag{60}$$

Therefore equation (58) is not valid as yet for values of k between 0 and $\frac{\Delta}{2}$. For such values, the second exponential term becomes real, and for negative values of $\underline{n}\cdot(\underline{r}'-\underline{r})$ the integral becomes divergent.

However, equation (58) may be extended for values of k given by $0 < k < (1/2)\Delta$, by demanding that the potential $U(\underline{r})$ should satisfy the restriction that

$$\int |U(r)| \, r \, e^{\kappa r} \, dr \quad \text{exists.*} \tag{61}$$

Here $a = 1/\kappa$ is the 'range' of the potential. Equation (61) means that $U(r)$ must fall off sufficiently fast. Hence the interpretation of κ . This condition is satisfied by a number of potentials. An additional restriction is

$$\Delta < 2\kappa \tag{62}$$

For practical pusposes, this is not a severe limitation because $a \sim 10^{-13}$, hence $\kappa \sim 10^{13}$ and the momentum transfer can assume values upto the order of 10^{13}.

The next step is to analytically continue the scattering amplitude $f(k, \Delta)$ to complex values of k . We denote the complex momentum by

$$z = k + i\beta \ , \quad \text{Im } z > 0 \ .$$

Then equation (58) is rewritten as

$$f(z, \Delta) = f_B(\Delta) + \iint T(z, \Delta) \, d^3\underline{r} \, d^3\underline{r}' \tag{63}$$

where

$$T(z, \Delta) = -\frac{1}{4\pi} \exp\left[-\tfrac{1}{2} i \underline{\Delta} \cdot (\underline{r} + \underline{r}')\right] \exp\left[i (z^2 - \tfrac{1}{4}\Delta^2)^{1/2} \underline{n} \cdot (\underline{r} - \underline{r}')\right]$$
$$U(r) \, g(\underline{r}, \underline{r}'; z) \, U(r') \tag{64}$$

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* This condition may be too stringent. In other words, it is a sufficient condition, but may not be a necessary one.

The physical scattering amplitude is given by

$$f(k, \Delta) = \lim_{\beta \to +0} f(z, \Delta) \tag{65}$$

The analytic properties of $f(z, \Delta)$ are determined by those of $T(z, \Delta)$. From equation (64) it appears as though a branch point exists at $z = (1/2)\Delta$. This is not so, because of the crossing symmetry of $f(k)$;

$$f(k) = \frac{1}{2}\left[f(k) + f^{x}(-k)\right] \tag{66}$$

whence the second exponential term in equation (64) reduces to $\cos\left[(k^2 - \frac{1}{4}\Delta^2)^{1/2}\ \underline{n}\cdot(\underline{r}'-\underline{r})\right]$. This, because of its evenness, has no branch points.

$T(z, \Delta)$ has poles in the upper half plane, since g_l has poles at $z = i\sqrt{|\epsilon_i|}$ in $\mathrm{Im}\ z > 0$, as evidenced by the bilinear expansion of g_l (see equation 53). This leads to the possibility of an essential singularity at ∞ for g_l, and hence for T. Hover, Bergmann* has shown that a finite number of poles exists only if

$$\int_0^\infty |U(r)|\ r\ dr \qquad \text{exists} \tag{67}$$

This further regulates the behaviour of $U(r)$ for small r.

Now consider the function

$$\frac{z'\ T(z', \Delta)}{z'^2 - z^2} \tag{68}$$

It has poles for $z' = i\sqrt{|\epsilon_i|}$, that is, at the poles of $T(z', \Delta)$. In addition, there are two poles at $z' = \pm z$ only one of which lies in the upper half of the z'-plane, and

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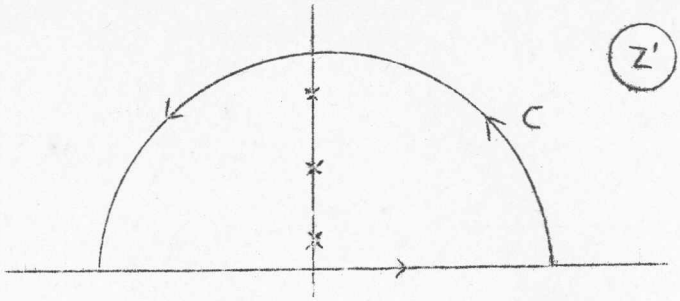
* Proc. Natl. Acad. Sci. U.S. 38, 961 (1952).

which is therefore of interest.



Let us draw a contour C in the z'-plane as shown, such that the semi-circle has a radius just large enough to enclose the pole farthest from the origin. Then Cauchy's integral formula gives

$$\frac{1}{2\pi i}\oint_C \frac{z'\,T(z',\Delta)}{z'^2 - z^2}\,dz' = \frac{1}{2}\,T(z,\Delta) + \sum_{i=1}^{N} \frac{z_i\,\Gamma(z_i)}{z_i^2 - z^2} \qquad (69)$$

where $\Gamma(z_i)$ is the residue of $T(z, \Delta)$ at the pole z_i, and N is the total number of poles of $T(z, \Delta)$ in the upper half plane

We define for convenience

$$\Gamma(z_i) = \frac{1}{2z_i}\,F_i(z_i) \qquad (70)$$

where, using equations (64) and (53), $F_i(z_i)$ is explicitly given by

$$F_i(z_i) = -\frac{1}{4\pi}\exp\left[-\frac{1}{2}\,\underline{\Delta}\cdot(\underline{r}+\underline{r}')\right]\exp\left[i\left(z_i^2 - \tfrac{1}{4}\Delta^2\right)^{1/2}\,\underline{n}\cdot(\underline{r}'-\underline{r})\right]$$
$$U(r)\,U(r')\,\varphi_i(\underline{r})\,\varphi_i^{*}(\underline{r}') \qquad (71)$$

Then equation (69) can be rewritten as

$$\frac{1}{\pi i}\oint_C \frac{z'\,T(z',\Delta)}{z'^2 - z^2}\,dz' = T(z,\Delta) + \sum_{i=1}^{N} \frac{F_i(z_i)}{z_i^2 - z^2} \qquad (72)$$

Integrating this over $\underline{r}$ and $\underline{r}'$ and rearranging terms

$$\iint T(z,\Delta)\,d^3\underline{r}\,d^3\underline{r}' = \frac{1}{\pi i}\iint d^3\underline{r}\,d^3\underline{r}'\oint_C \frac{z'\,T(z',\Delta)}{z'^2 - z^2}\,dz'$$
$$+ \sum_{i=1}^{N} \frac{R_i(z_i\,\Delta)}{z^2 - z_i^2} \qquad (73)$$

where $$R_i(z_i,\Delta) = \int\int F_i(z_i)\, d^3\underline{r}\, d^3\underline{r}' \tag{74}$$

substituting from equation (73) in equation (63):

$$f(z,\Delta) = f_B(\Delta) + \sum_{i=1}^{N} \frac{R_i(z_i,\Delta)}{z^2 - z_i^2} + \frac{1}{\pi i}\int\int d^3\underline{r}\, d^3\underline{r}' \oint \frac{z' T(z'\Delta)}{z'^2 - z^2}\, dz' \tag{75}$$

It can be proved* that the integrations $\int\int d^3\underline{r}\, d^3\underline{r}'$ and $\oint_C dz'$ can be interchanged. (This means that the integral must converge uniformly with respect to z'.) Then equation (75) becomes

$$f(z,\Delta) = f_B(\Delta) + \sum_{i=1}^{N} \frac{R_i(z_i\Delta)}{z^2 - z_i^2} + \frac{1}{\pi i}\oint_C \frac{z'\left[f(z',\Delta) - f_B(\Delta)\right]}{z'^2 - z^2}\, dz' \tag{76}$$

This is not yet a dispersion relation since the contour C is not an infinite one. The contribution from an infinite semi-circle can be shown ** to be zero, that is, ρ_i and hence $T(z, \Delta)$ obey the asymptotic conditions, provided that the potential $U(r)$ obeys the conditions given in (61) and (67). These conditions, however, have already been stipulated. Therefore in equation (76) the contour integral may be replaced by an integral along the real axis;

$$\oint \frac{z'\left[f(z'\Delta) - f_B(\Delta)\right]}{z'^2 - z^2}\, dz' = \int_{-\infty}^{\infty} \frac{k'}{k'^2 - k^2}\left[f(k',\Delta) - f_B(\Delta)\right] d$$

Since the Born term $f_B(\Delta)$ is antisymmetric in k', it does not contribute to the integral. Also by using the crossing symmetry of $f(k', \Delta)$, the limits of integration may be changed

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* [illegible] and Zemach, Ann. Phys. 7, 440 (1959) appendix.

** A. Klein and C. Zemach, Ann. Phys. 7, 440, (1959) Appendix.

and the integral written as

$$2i \int_0^\infty \frac{k'}{k'^2 - k^2} \, \mathrm{Im}\, f(k', \Delta)\, dk'$$

Therefore equation (76) is finally,

$$f(z,\Delta) = f_B(\Delta) + \sum_{i=1}^{N} \frac{R_i(z_i,\Delta)}{z^2 - z_i^2} + \frac{2}{\pi} \int_0^\infty \frac{k' \, \mathrm{Im}\, f(k',\Delta)}{k'^2 - k^2} \, dk' \qquad (77)$$

It must be remembered that this is valid only in the region Im $z > 0$. Thus $f(z, \Delta)$ can be calculated knowing the eigenvalues $z_i^2 = -|\varepsilon_i|$ and the eigenfunctions φ_i.

The computation of the Ri may be complicated. In the simplest case, when $\Delta = 0$, Ri is uniquely determined by the asymptotic normalization constant of the bound state φ_i. When $\Delta \neq 0$, then Ri is real and finite as long as $\Delta < 2\kappa$

When z is real, that is, for real momentum, equation (77) must be modified to

$$f(k,\Delta) = f_B(\Delta) + \sum_{i=1}^{N} \frac{R_i(z_i,\Delta)}{k^2 + |\varepsilon_i|} + 2/\pi \lim_{\beta \to 0} \int_0^\infty \frac{k' \, \mathrm{Im}\, f(k',\Delta)\, dk'}{k'^2 - (k+i\beta)^2} \qquad (78).$$

Reformulation of Dispersion Relation in Terms of Energy.

It is useful to rewrite the dispersion relation in terms of energy as the dispersed variable. We therefore introduce the square of the complex momentum

$$s = z^2 \tag{79}$$

The quantity $\frac{\hbar^2}{2m} s$ represents the complex energy.

We also define $t = \Delta^2$

$$= 2s(1 - \cos\vartheta) \tag{80}$$

Recalling $z_i = i\sqrt{|\epsilon_i|}$ (77) is rewritten as

$$f(s,t) = f_B(t) + \sum_{i=1}^{N} \frac{R_i(|\epsilon_i|,t)}{s+|\epsilon_i|} + \frac{1}{\pi}\int_0^\infty \frac{Im\, f(s',t)}{s'-s}\, ds' \tag{81}$$

This is of course valid for all s for which $Im\, s \neq 0$

When s is real, equation (81) is modified to

$$f(s,t) = f_B(t) + \sum_{i=1}^{N} \frac{R_i(|\epsilon_i|,t)}{s+|\epsilon_i|} + \lim_{\eta\to+0} \frac{1}{\pi}\int_0^\infty \frac{Im\, f(s',t)}{s'-s-i\eta}\, ds' \tag{81a}$$

This is valid for all points on the s-plane except for the poles at $s = -|\epsilon_i|$ and the cut from $s = 0$ to $s = \infty$ along the real axis. The conditions to be observed are

$$\left.\begin{aligned} &\int_0^\infty |U(r)|\, r\, e^{\kappa r}\, dr \quad \text{exists} \\ &\int_0^\infty |U(r)|\, r\, dr \quad \text{exists} \end{aligned}\right\} \tag{82}$$

and

$$t < 4\kappa^2 \quad (\text{i.e.} \quad \Delta < 2\kappa) \tag{83}$$

If the potential decreases faster than any exponential, then κ can become equal to ∞, and there is no restriction on t (or Δ). For example cut potentials do not have any restriction on t. However the Yukawa potential does have a limitation since in this case κ is infinitesimally greater than the coefficient of the exponent in the expression for the potential.

We shall now consider the real part of $f(s,t) - f_B(t)$ Since the R_i are real,

$$Re\left[f(s,t) - f_B(t)\right] = \sum_{i=1}^{N} \frac{R_i(|\epsilon_i|,t)}{s+|\epsilon_i|} + \frac{P}{\pi}\int_0^\infty \frac{Im\, f(s',t)}{s'-s}\, ds' \qquad (34)$$

If we take the imaginary part of (81a) we end up with a trivial identity

Im f (s , t) = Im f (s , t)

Equation (84) as a dispersion relation was derived without making any subtractions. Hence (as also seen from equation 82) f (s , t) - f_B (t) $\to$ 0 as $|s| \to \infty$. We notice that the scattering amplitude itself does not go to zero as $|s| \to \infty$. This only emphasizes the usefulness of the first Born approximation. Even if the Born series does not converge, the first Born approximation is good enough at high energies.

Forward Scattering:

In the case of forward scattering, the 'Optical Theorem' states that

$$\text{Im } f(s, 0) = \frac{\sqrt{s}}{4\pi} \sigma(s) \quad , \quad s > 0 \qquad (85)$$

The dispersion integral could be evaluated if we know $\sigma(s)$ for $s = 0$ to $s = \infty$. Also, it is easy to compute R_i when $t = 0$.

It can be shown* that R_i is completely determined by the asymptotic normalization coefficients of the corresponding bound state eigenfunctions φ. Hence the forward scattering amplitude $f(s, 0)$ can be calculated. This is the simplest application of the dispersion relations. The theory thus relies essentially on experimental data; the approach is free from the operator formalism of Quantum Theory. Thus the theory of the dispersion relations is an alternative approach to the problem of interaction.

Non-Forward Scattering:

Even if $t \neq 0$, it is possible to show that R_i is real and a polynomial in t:

$$R_i(|\epsilon_i|, t) = \sum_{m=0}^{\ell} a_m(|\epsilon_i|)\, t^m \qquad (86)$$

where ℓ is the angular momentum of the bound state for which the energy is $|\epsilon_i|$.

Now the equation arises as to what kind of experimental data can be fed into the dispersion relations in the case of non-forward scattering. Here we encounter a difficulty characteristic

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* Ref: for example, M.L.Goldberger's review article in Relations de Dispersion at particules Elementaires, John Wiley and Sons, Inc.

of both relativistic and non-relativistic dispersion theory. The integral in equation (34) covers the entire range from $s = 0$ to $s = \infty$. However equation (30) demands that for physical angles, that is, for $|\cos\theta| < 1$,

$$s' > (1/4)\, t \tag{87}$$

Therefore Im $f(s', t)$ cannot be determined experimentally for the range

$$0 \leq s' < (1/4)t \tag{88}$$

Hence the function Im $f(s', t)$ has to be analytically continued into this 'unphysical'region, and this is done by using the expansion:

$$f(s,t) = \frac{1}{\sqrt{s}} \sum_{\ell=0}^{\infty} (2\ell+1)\, e^{i\delta_\ell(s)} \sin\delta_\ell(s)\, P_\ell\left(1 - t/2s\right), \quad s > 0 \tag{89}$$

For the unphysical region, the modulus of the argument of P_ℓ is greater than 1. Then $f(s, t)$ for the unphysical region can be found only if the series in equation (89) converges. To find if this is so, we make use of the following theorem in analysis:

If $G(\theta)$ is on analytic function of θ in the complex $\cos\theta$ plane within an ellipse with foci at ± 1, then $G(\theta)$ can be expanded inside the ellipse in terms of Legendre polynomials:

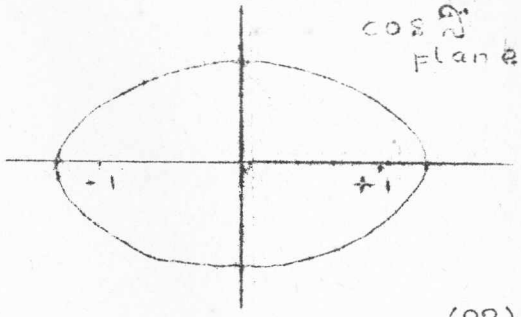
$$G(\theta) = \sum_{\ell=0}^{\infty} C_\ell\, P_\ell\, (\cos\theta) \tag{90}$$

We must therefore have an ellipse in the complex $\cos\theta$ plane inside which Im $f(s, t)$ is analytic. Such an ellipse does exist and is called the Lehmann ellipse. It can be found by expressing f in terms of the Green's function and utilizing the

partial wave decomposition* . Its semi-major and semi-minor axes are given by

$$a = 1 + 2k^2/s$$
$$b = (a^2 - 1)^{1/2} \qquad (91)$$

So the extension of Im $f_1(s', t)$ in the unphysical region is possible for real $\cos\vartheta$ if



$$|\cos\vartheta| < 1 + 2\frac{k^2}{s'} \qquad (92)$$

that is, if $-\left(1 + \frac{2k^2}{s}\right) < \left(1 - t/2s\right) < \left(1 + \frac{2k^2}{s}\right)$

or

$$-4k^2 < t < 4k^2 + 4s \qquad (93)$$

Since we are interested for values of s down to $s = 0$, the condition

$$t < 4k^2$$

This is precisely the condition already demanded in (83). Therefore no new condition is necessary to expand $f(s', t)$ in a Legendre series. Hence

$$\text{Im } f(s', t) = \sum_{l=0}^{\infty} a_l(s') P_l\left(1 - \frac{t}{2s}\right), \quad t < 4k^2 \qquad (94)$$

The coefficients $a_l(s')$ can be obtained by employing the orthogonality properties of Legendre polynomials.

$$a_l(s') = \frac{2l+1}{4s'} \int_0^{4s'} P_l\left(1 - \frac{t}{2s'}\right) \text{Im } f(s', t)\, dt \qquad (95)$$

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* See A. Klein and C. Zemach, ibid (1959).

Since the range of integration $0 \leq t \leq 4s$ is physically accessible, Im $f(s, t)$ can be experimentally determined, and hence a_l calculated. In practice the calculations are extremely tedious and approximations are made by taking only the first few partial wave terms.

We note here that the condition for the Legendre expansion of $f(s, t)$ is really

$$t < k^2$$

This is due to the Born term $f_B(t)$. It is only $(f - f_B)$ which can be expanded subject to the condition $t < 4k^2$. Since the Born term is real, equation (94) is valid only for $t < k^2$.

It may be possible, for small t, to extrapolate Im $f(s', t)$ to the unphysical region $0 < s < (1/4)t$ from measurements in the physical region $(1/4)t < s < \infty$. However, such a procedure is unreliable since a small error in measurements may lead to large errors in the extrapolation region. Such extrapolation becomes unavoidable in some cases, e.g. K-N scattering. On the other hand, for π - N scattering the function in the unphysical region can be determined theoretically.

Remarks on Analytic Propertoes of $f(s, t)$.

The scattering amplitude $f(s, t)$ in analytic every where on the s-plane, with a cut along the real axis from $s = 0$ to $s = \infty$, except for the poles $s = -|\epsilon_i|$. The poles signify bound states, while the positive cut, the scattering states. These singularities arise from the bilinear expansion of the Green's function, which is valid for Im $z > 0$, which corresponds to the first Riemann sheet i.e., Im $\sqrt{s} > 0$.

The analytic behaviour of $f(s, t)$ in the second Riemann sheet defined by $\mathrm{Im}\ \sqrt{s} < 0$ is best studied in terms of the momentum variable z for $\mathrm{Im}\ z < 0$. But Stone's theorem, and consequently the bilinear formula given earlier, are not valid for $\mathrm{Im}\ z < 0$. A much more complicated investigation* shows that there may be an infinite number of poles in the lower half of the complex momentum plane. Those which do not lie on the negative imaginary axis occur in pairs symmetric with respect to this axis.

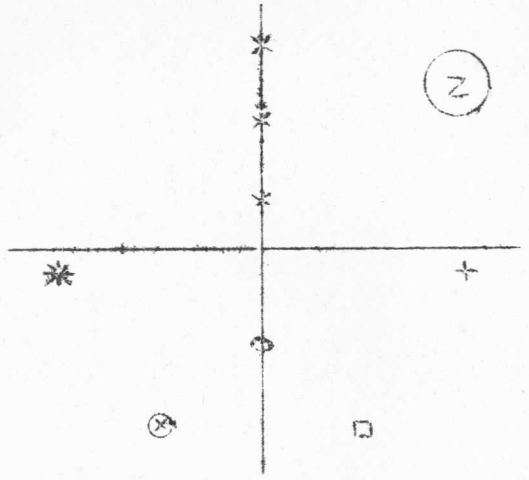

Fig (a)

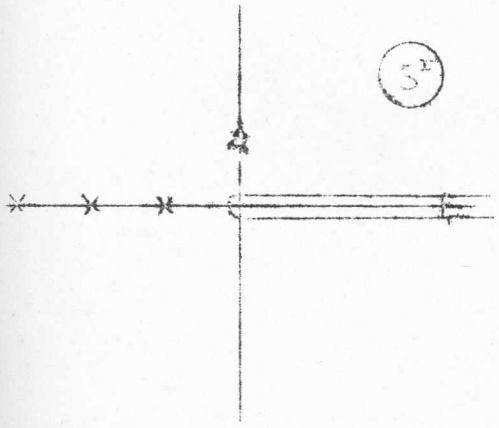

Fig (b)

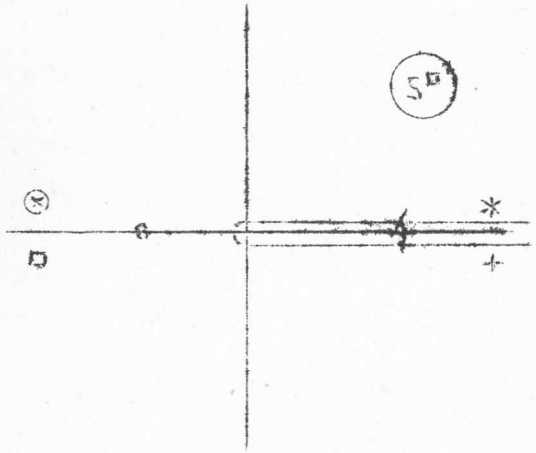

Fig (c)

* R. G. Newton, Journ. Math. Phys. 1, 319 (1960).

Figure (a) indicates all the types of poles on the z plane; figures (b) and (c) indicate the corresponding poles on the appropriate Riemann sheets. The poles on the second Riemann sheet s^{II} have the following physical interpretation.

The pole denoted by + in the fourth quadrant of the plane corresponds to decaying (metastable) state with positive energy. Let it be represented by $E_1 - i E_2$. Then the expression

$$e^{-ist} = e^{-E_1 t} \; e^{-E_2 t}$$

exhibits the decay with $E_2 = 1/(\text{lifetime})$. When E_2 is small the state appears as a resonance in the scattering amplitude at $s \approx E_1$. For a resonance,

$$f(s, t) \approx \frac{2\ell+1}{k} \; \frac{\Gamma/2}{E_r - E - i\,\Gamma/2} \qquad (96)$$

By comparison, we note that $E_1 = E_r$ and $E_2 = -\Gamma/2$ where E_r is the resonance energy and $\Gamma/2$ the half width of the resonance.

Next, the pole shown as * has a positive imaginary part. This can be interpreted as a capture process, which however does not last long; the incident particle is scattered after a short lapse of time. Actually, a resonance is caused by the combined action of the * and + poles.

The poles ⊡ and ⊗ have no clear physical interpretation.

The pole denoted by 0 signifies a 'virtual' bound state. This is because the energy has no imaginary part which might have caused instability. However, $\text{Im}\sqrt{s} < 0$. If this virtual bound state (often called also an 'anti-bound state') lies near to the origin, it may cause a near-zero energy resonance and

dominate the low energy scattering, just as much as a very low lying real bound state would.

When a pole coincides with the branch point it is interpreted as zero energy resonance scattering. If the potential consists of a strong and a weak part, and if we neglect the latter, then we have a pole on the cut signifying a discrete state in the scattering states. However, the presense of the weak part displaces it slightly below the real axis. This can be interpreted as a radioactive decaying state. In experiments this is observed as a resonance. It differs from other resonances in that its decay is not pure exponential.

Chapter IV.

THE MANDELSTAM REPRESENTATION FOR POTENTIAL SCATTERING

Hitherto the scattering amplitude was treated as a function of fixed momentum transfer (subject to $t < 4k^2$) and variable energy, s. Now the question arises whether the restriction on t is a consequence of the particular way in which the dispersion relation was arrived at, or whether it is the natural boundar for the analyticity of the scattering amplitude. Further we may investigate f as a function of both s and t. To do this we first consider f as a function of t for fixed s, ($s > 0$). With the aid of the dispersion relation thus obtained we write down the scattering amplitude with both s and t as arbitrary complex variables. This is precisely the Mandelstam Representation

The Mandelstam Representation plays an important role in the theory of elementary particles*. It provides a noval approach to the study of strong interactions. Nevertheless it cannot be rigorously proved in Relativistic Quantum Field Theory. In potential scattering theory on the other hand, its scope is limited. Yet, considerable insight can be gained by pursuing the problem the problem in potential scattering.

We have already seen that for fixed t and arbitrary s, Im f (s, t) can be expanded inside the Lehmann ellipse in a Legendre series provided t satisfies,

$$-4k^2 < t < 4k^2 + 4s$$

The expansion is not valid outside the ellipse because of a singularity on the periphery of the ellipse. This in fact corresponds to the branch point at $t = -4k^2$. Therefore we must

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* G.F.Chew, S-Matrix Theory of Strong Interactions, W.A.Benjamin, Inc.

introduce a branch cut in the t-plane from $t = -4\kappa^2$ to $t = -\infty$. Now we can expand the scattering amplitude in the cut t-plane, but the expansion need not be a Legendre series. To prove that such an expansion is possible we return to equation (58);

$$f(s,t) - f_B(t) = -\frac{1}{4\pi}\iint e^{-\frac{1}{2}\Delta\cdot(\gamma+\gamma')} e^{i(k^2-\frac{1}{4}\Delta^2)\eta\cdot(\gamma-\gamma')} U(r) f_n(r,r';k) U(r') d^3r\, d$$

This equation is, essentially, a Fredholm type integral equation whose solution may be expressed as a series, each term of which is a function of t. It can be shown that, under rather wide conditions, each term of the series is analytic in the cut t-plane and also that the series converges uniformly. Hence the required analytic continuation is possible*.

For example, we consider potentials U(r) which are superpositions of Yukawa potentials

$$U(r) = \int_{\kappa}^{\infty} \sigma(\mu)\, \frac{e^{-\mu r}}{r}\, d\mu \qquad (97)$$

where $1/\kappa$ is the maximum range of the potential. But U(r) is already required to satisfy the condition given by equation (82). This demands that $\sigma(\mu)$ should satisfy the following restrictions:-

(1) $\sigma(\mu)$ is bounded function with possible δ-function singularities.

(2) $\sigma(\mu)/\mu \to 0$ as $\mu \to 0$.

and (3) $\sigma(\mu) \to 0$ as $\mu \to \infty$

This assumed potential encompasses many kinds of potentials including the Yukawa and the Gaussian potentials. (However,

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* R.Blankenbecler et al: Ann.of Phys. 10, 62 (1960).

for cut-off forms like the square well potential, the analyticity of $f(s, t) - f_B(t)$ does not hold.)

Incidentally, though the function $f(s, t) - f_B(t)$ is analytic in the t-plane with a cut from $t = -4\kappa^2$ to $t = -\infty$ the function $f(s, t)$ itself is not so. This is due to the Born term, which may be calculated using equation (97). We then have

$$f_B(t) = -\int_{\kappa}^{\infty} \frac{\sigma(\mu)}{t+\mu^2}\, d\mu$$

This shows that for the Born term the cut begins at $t = -\kappa^2$ so that for $f(s, t)$ the cut lies between $t = -\kappa^2$ and $t = -\infty$.

Let us examine equation (82) again:

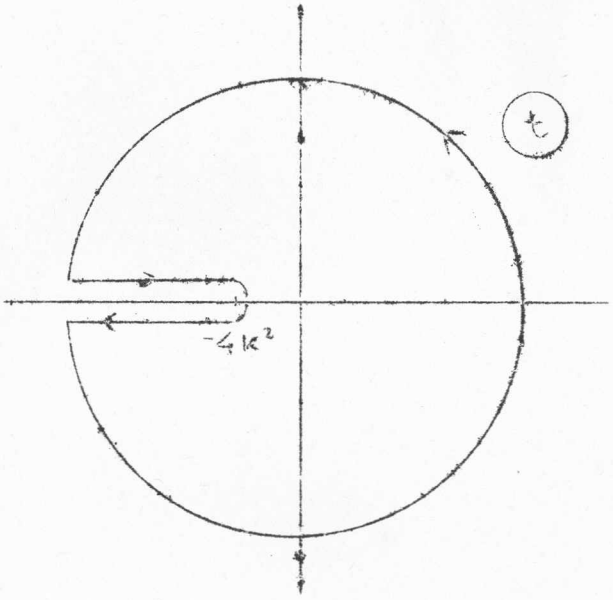
$$f(s,t) - f_B(t) = \sum_{i=1}^{N} \frac{R_i(|G_i|, t)}{s + |\epsilon_i|} + \frac{1}{\pi} \lim_{\eta \to 0} \int_{0}^{\infty} \frac{\mathrm{Im}\, f(s',t)}{s' - s - i\eta}\, ds'$$

On the left, the function $f - f_B$ has been proved to be analytic in the cut t-plane. On the right hand side, the function R_i is a polynomial in t. Therefore it must be analytic everywhere in the t-plane, except for the pole of order ℓ at $t = \infty$ if the highest power of t in the polynomial is ℓ. The last term involving the integral was shown to be valid for arbitrary s and t in the range $0 < t < 4\kappa^2$. But now we make use of a theorem which states that if two functions (in our case, the left hand side and the right hand side of the equation) are analytic in two domains, and if the domains, overlap in one region, then each function is an analytic continuation of the other in its own domain.

We can therefore extend the last term in the above equation to all values of t.

The function Im f (s', t) will now have to be explicitly stated in terms of known functions. Since nothing is known about its behaviour at infinity, let us initially assume that

$$\text{Im } f(s', t) \to 0 \text{ as } |t| \to \infty, \quad s' \geq 0$$



Then Cauchy's theorem may be used to find Im f (s', t) by integrating $\oint \frac{\text{Im } f(s',t')}{t'-t}\, dt'$ along the contour shown. The contribution due to the circle at infinity vanishes, and we are left with

$$\text{Im } f(s',t) = \lim_{\gamma \to 0} \frac{1}{2\pi i} \left[\int_{-\infty}^{-4\kappa^2} \frac{\text{Im } f(s',t'+i\gamma)}{t'-t}\, dt' + \int_{-4\kappa^2}^{-\infty} \frac{\text{Im } f(s',t'-i\gamma)}{t'-t}\, dt' \right]$$

$$= \frac{1}{\pi} \int_{-\infty}^{-4\kappa^2} \frac{u_s(s',t')}{t'-t}\, dt'$$

where u is the discontinuity across the cut. This is rewritten in terms of the discontinuity function $\rho(s', t')$ given by

$$\rho(s',t') = -u(s',-t')$$

$$= \frac{1}{2i} \lim_{\varepsilon \to 0} \left[\mathrm{Im}\, f(s',-t'-i\varepsilon) - \mathrm{Im}\, f(s',-t'+i\varepsilon) \right] \tag{98}$$

Hence

$$\mathrm{Im}\, f(s',t) = \frac{1}{\pi} \int_{4k^2}^{\infty} \frac{\rho(s',t')}{t'+t}\, dt' \tag{99}$$

Now the functional form of Im f(s', t') is obtained by taking the imaginary part of f (s', t') when s' and t' are real. When s' and t' take complex values, then Im f(s', t') itself will, in general, have real and imaginary parts. However, we know that for $t > -4k^2$, Im f(s', t') is real, and therefore using Schwartz's reflection principle,

$$\left[\mathrm{Im}\ f(s', t') \right]^{*} = \mathrm{Im}\ f(s', t'^{*})$$

Hence the term in brackets in equation (98) is pure imaginary and therefore ρ (s', t') is real.

In the more general case, let Im f(s', t) obey the condition Im f (s', t) → a polynomial in t of degree n as $|t| \to \infty$.

In this case, Im f (s', t) is given by

$$\mathrm{Im}\, f(s',t) = (-1)^{n+1} \frac{z^{n+1}}{\pi} \int_{4k^2}^{\infty} \frac{\rho(s',t')}{(t'+t)\, t'^{n+1}}\, dt'$$

$$+ \sum_{j=0}^{n} \frac{t^j}{j!}\, q_j(s') \tag{100}$$

Here the subtractions have been made at t = 0 and

$$q_j(s') = \left[\frac{\partial^j}{\partial t^j} \mathrm{Im}\, f(s',t) \right]_{t=0}.$$

However the exact value of n is unknown, except that $n \geq \ell + 1$ where ℓ is the maximum angular momentum quantum number.

Suppose now that there are no bound states and that no subtractions are necessary. Then using equations (82) and (99),

$$f(s,t) - f_B(t) = \frac{1}{\pi^2} \lim_{\eta \to 0} \int_0^\infty \int_{4\kappa^2}^\infty \frac{\rho(s',t')\, dt'\, ds'}{(s'-s-i\eta)(t'+t)} \qquad (101)$$

This is the Mandelstam representation for the full scattering amplitude for potential scattering, valid for all complex values of s and t except for the cut in the t-plane.

In the more general case, where there are N poles and $(n+1)$ subtractions to be performed, we have, using equations (82) and (100)

$$f(s,t) - f_B(t) = \sum_{i=1}^{N} \frac{R_i(|\epsilon_i|, t)}{s + |\epsilon_i|}$$

$$+ (-1)^{n+1} t^{n+1} \frac{1}{\pi^2} \lim_{\eta \to 0} \int_0^\infty \int_{4\kappa^2}^\infty \frac{\rho(s',t')\, ds'\, dt'}{(t'+t)\, t'^{n+1} (s'-s-i\eta)}$$

$$+ \sum_{j=0}^{n} \frac{t^j}{j} \frac{1}{\pi} \lim_{\eta \to 0} \int_0^\infty \frac{g(s')\, ds'}{s'-s-i\eta} \qquad (102)$$

Again, this Mandelstam representation or 'double dispersion relation' is valid for all s and t, except for the cut in the t-plane.

Thus the analytic function $f(s, t)$ is completely determined by the singularities of $f(s, t)$ in the s and t planes.

An analogy can be drawn from electrostatics. There the potential due to a distribution of charges is completely determined by the positions of the point charges (poles) and line charges (cut in t-plane). The analogy must not be carried too far, since in our case the poles and the cut arise from different variables.

Equation (101) contains as a special case, the dispersion relations for $f(s, t)$ with s fixed and t variable, or with t fixed and s variable. For example, taking imaginary parts of both sides of the equation, we obtain (keeping s and t real):

$$\text{Im } f(s, t) = \frac{1}{\pi} \int_{4\kappa^2}^{\infty} \frac{\rho(s, t')}{t' + t} \, dt' \qquad (103)$$

Similarly taking real parts

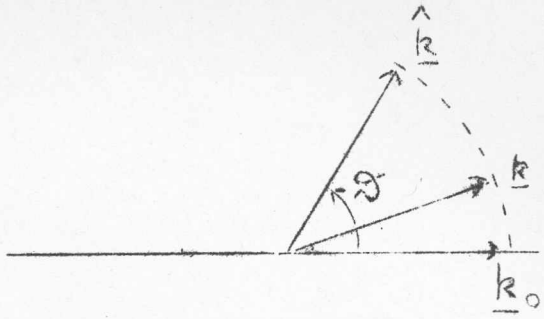
$$\text{Re } \left[f(s, t) - f_B(t) \right] = \frac{1}{\pi} P \int_{0}^{\infty} \frac{\text{Im } f(s', t) \, ds'}{s' - s} \qquad (104)$$

We appear to have recovered equation (99) and (84). But the Mandelstam representation shows that these relations hold not merely for real s and real t, but also, by analytic continuation, for any arbitrary s and t.

Calculation of $\rho(s, t)$:

Finally, we note that the functions ρ and g appearing in equations (101) and (102) are yet unknown. Since ρ is defined in terms of Im $f(s, t)$ and vice versa, it is obvious that another relation between the two must be introduced in order to determine ρ. This is the unitarity condition for potential scattering:

$$\text{Im } f(s, t) = \frac{\sqrt{s}}{4\pi} \int f^{*}(s, t_1) \, f(s, t_2) \, d\Omega' \qquad (105)$$



where $t = (\underline{k} - \underline{k}_0)^2$

$t_1 = (\underline{k} - \underline{k})^2$

$t_2 = (\underline{k} - \underline{k}_0)^2$

and $d\Omega' = \frac{1}{k^2} d^3\underline{k}$

The integration is carried out over all orientations of $\underline{k}$.

If $t = 0$, then equation (105) reduces to the optical theorem.

As it stands, equation (105) is valid only for real s and for $t < 4k^2 + 4s$. But the Mandelstam representation enables us to see that both sides of the equation can be extended to arbitrary complex values of s and t. Therefore equation (101) may be substituted in (105) to yield:

$$\mathrm{Im}\, f(s,t) = \frac{\sqrt{s}}{4\pi} \int d\Omega' \left[f_B(t_1) + \frac{1}{\pi^2} \lim_{\eta \to 0} \iint \frac{\rho(s',t')\, dt'ds'}{(s'-s+i\eta)(t'+t_1)} \right] \left[f_B(t_2) + \frac{1}{\pi^2} \lim_{\eta \to 0} \iint \frac{\rho(s'',t'')\, dt''ds''}{(s''-s-i\eta)(t''+t_2)} \right] \tag{106}$$

Let us now restrict the potential to a simple Yukawa potential

$$U(r) = \lambda \frac{e^{-\kappa r}}{r} \tag{107}$$

where λ is the strength parameter. The Born term then works out to

$$f_B(t) = -\frac{\lambda}{t + \kappa^2}$$

Substituting this in equation (106), the right hand side can be seen to contain the following integrals:

$$\int d\Omega' \frac{1}{(t_1+K^2)(t_2+K^2)} \quad ; \quad \int d\Omega' \frac{1}{(t_1+K^2)(t_2+t'')}$$

$$\int d\Omega' \frac{1}{(t_2+K^2)(t_1+t')} \quad ; \quad \int d\Omega' \frac{1}{(t_1+t')(t_2+t'')}$$

These integrals can be written most generally as

$$\bar{I}_n = \int d\Omega' \frac{1}{(t_1+\alpha)(t_2+\beta)} \tag{108}$$

where α and β stand for K^2, t', or t'', depending upon the choice of the integral.

We now introduce

$$\tau_1 = 1 + \frac{\alpha}{2s}$$
$$\tau_2 = 1 + \frac{\beta}{2s} \tag{109}$$

Using these quantities, (108) becomes

$$\bar{I}_n = \frac{1}{4s^2} \int d\Omega' \frac{1}{\left(\tau_1 - \frac{\underline{k}\cdot\underline{k}}{k^2}\right)\left(\tau_2 - \frac{\underline{k}\cdot\underline{k}_0}{k^2}\right)} \tag{110}$$

It is possible to re-express this integral as

$$\bar{I}_n = \frac{\pi}{s^2} \int_{b_n}^{\infty} \frac{1}{v+t} \frac{1}{A_n(\xi)} dv \tag{111}$$

where $\xi = 1 + \frac{\upsilon}{2s}$

$$\left.\begin{aligned} A_n(\xi) &= \left[(\tau_1\tau_2 - \xi)^2 - (\tau_1^2-1)(\tau_2^2-1)\right]^{1/2} \\ \ell_{\upsilon_n} &= 2s\left\{\tau_1\tau_2 - 1 + \left[(\tau_1^2-1)(\tau_2^2-1)\right]^{1/2}\right\} \end{aligned}\right\} \quad (112)$$

We also introduce the step function $\theta(\upsilon - \ell_{\upsilon_n})$ defined by

$$\theta(\upsilon-\ell_{\upsilon_n}) = \begin{cases} 1 & \text{if } \upsilon \geq \ell_{\upsilon_n} \\ 0 & \text{if } \upsilon < \ell_{\upsilon_n} \end{cases} \quad (113)$$

The limits in (111) can be changed so as to read:

$$I_n = \frac{\pi}{2s^2}\int_0^\infty \frac{\theta(\upsilon-\ell_{\upsilon_n})}{\upsilon+t}\,\frac{1}{A_n(1+\upsilon/2s)}\,d\upsilon \quad (114)$$

With this form of I_n in mind, equation (106) is rewritten:

$$\begin{aligned} \overline{I}_m f(s,t) = \frac{1}{4s^{3/2}}\int_0^\infty \frac{d\upsilon}{\upsilon+t}\Bigg[& \lambda^2\,\frac{\theta(\upsilon-\ell_{\upsilon_1})}{A_1(1+\upsilon/2s)} \\ & - \frac{\lambda}{\pi^2}\lim_{\eta\to 0}\iint \frac{\theta(\upsilon-\ell_{\upsilon_2})}{A_2(1+\upsilon/2s)}\,\frac{\rho(s',t')\,dt'ds'}{s'-s+i\eta} \\ & - \frac{\lambda}{\pi^2}\lim_{\eta\to 0}\iint \frac{\theta(\upsilon-\ell_{\upsilon_3})}{A_3(1+\upsilon/2s)}\,\frac{\rho(s'',t'')\,dt''ds''}{s''-s-i\eta} \\ & + \frac{1}{\pi^4}\lim_{\eta\to 0}\iiint \frac{\theta(\upsilon-\ell_{\upsilon_4})}{A_4(1+\upsilon/2s)}\,\frac{\rho(s',t')\rho(s'',t'')\,dt'ds'dt''}{(s'-s+i\eta)(s''-s-i\eta)} \end{aligned} \quad (115)$$

(115)

This unwieldly relation, gives the function Im f(s, t) for complex s and t . Our aim is to find the discontinuity $\rho(s, t)$ across the cut in the t-plane. To do this we use a limiting procedure:

$$\rho(s,t) = \frac{1}{2i} \lim_{\gamma \to 0} \left[\mathrm{Im}\, f(s, t+i\gamma) - \mathrm{Im}\, f(s, t-i\gamma) \right]$$

Doing this and recapitulating the relations (109), (112), the weight function is written

$$\rho(s,t) = \lambda^2 K(s,t;k^2,k^2) - 2\frac{\lambda}{\pi^2} P\int_0^\infty \int_{4k^2}^\infty \frac{K(s,t;t',k^2)}{s'-s} \rho(s',t')\, dt' d$$

$$+ \frac{1}{\pi^4} \lim_{\eta \to 0} \int_0^\infty \int_{4k^2}^\infty \int_0^\infty \int_{4k^2}^\infty \frac{K(s,t;t't'')}{(s'-s+i\eta)(s'-s-i\eta)} \rho(s',t')\rho(s'',t'')\, dt''\, ds''\, dt'\, ds'$$

(116)

where

$$K(s,t,a,b) = \frac{\pi}{2}\, \theta\left[t-a-b-\frac{ab}{2s} - \frac{\sqrt{ab}}{2s}\left\{ 16s^2 + 4s(a+b) + ab \right\}^{1/2} \right]$$

$$\left[s\left\{ t-(\sqrt{a}+\sqrt{b})^2 \right\}\left\{ t-(\sqrt{a}-\sqrt{b})^2 \right\} - t\,ab \right]$$

(117)

We now have a non-linear integral equation for $\rho(s, t)$. It is non-linear because of the last term. With the solution we can calculate the weight function for real and positive t and thus use it in the Mandelstam representation.

Equation (116) can be solved for $\rho(s, t)$ to any desired degree of approximation, at least in principle. This is done by means of the ''strip approximation''.

It is to be noted first that because each term on the right hand side contains a θ-function, any of the terms contributes only if a certain relation is satisfied. For example, the first term will contribute provided

$$K(s, t; \kappa^2, \kappa^2) \neq 0 ,$$

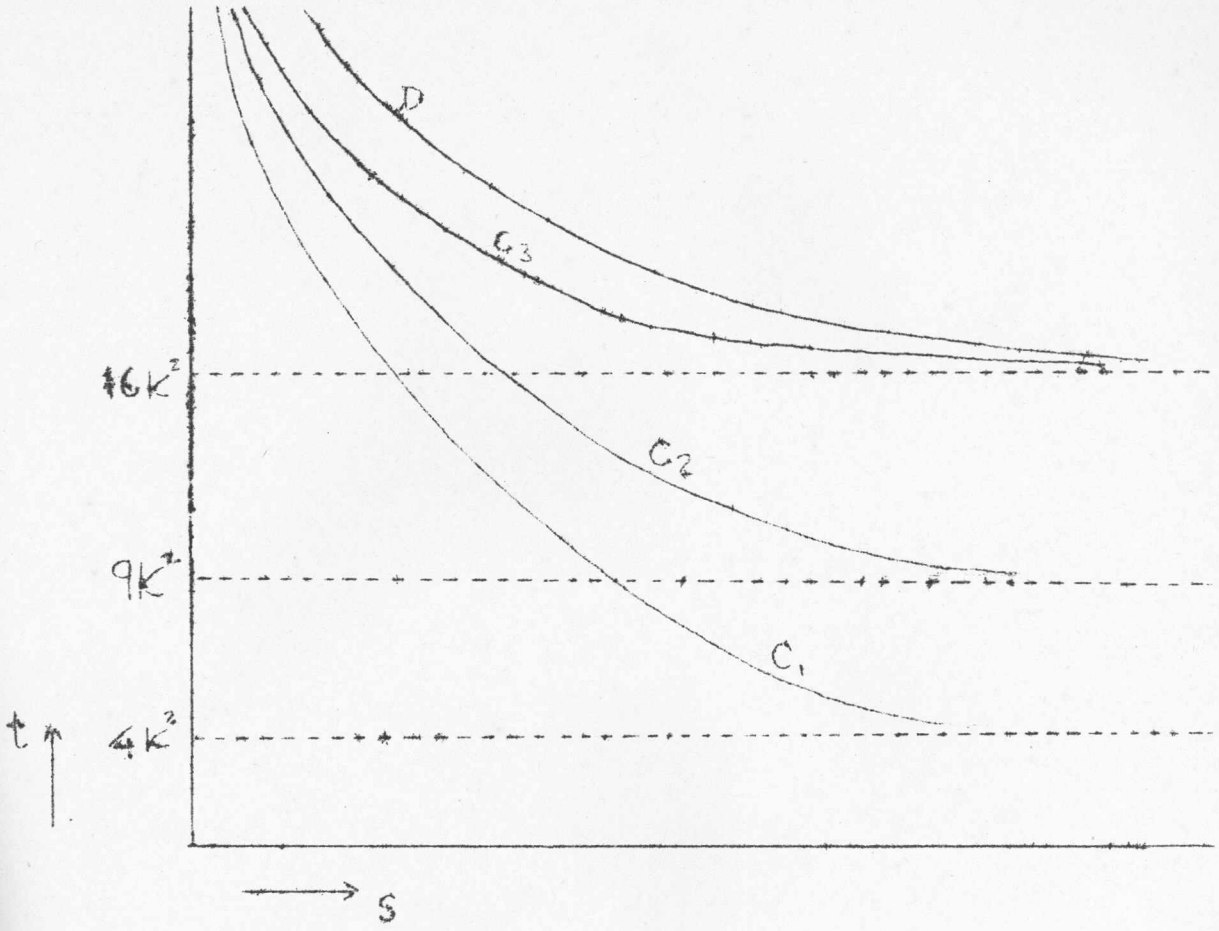
that is to say, provided the argument of the θ-function is positive. This requires that

$$t > 4\kappa^2 + \frac{\kappa^4}{s} \qquad (118)$$

One may visualise a curve C_1 drawn in the s - t plane (both s and t real and positive):

$$st - 4\kappa^2 s - \kappa^4 = 0 \qquad (119)$$

Then the first term in (116) exists only if the s and t values define a point lying above this curve.



It can be seen from (118) that the minimum value of t must be $4K^2$

In general, equation (117) shows that for a curve like C_1

$$t \approx \frac{ab}{s} \quad \text{for small } s$$

$$t \approx \left(\sqrt{a} + \sqrt{b}\right)^2 \quad \text{for large } s.$$

Similarly, the second term in (116) makes a contribution only if the kernel $K(s, t; t', K^2)$ is non-zero. Since the lower limit of integration over t' is $4K^2$, this condition is

$$K(s, t; 4K^2, K^2) \neq 0.$$

The curve so obtained is defined by

$$s(t - 9K^2)(t - K^2) - 4K^2 t = 0. \qquad (120).$$

Let this be denoted by C_2. The minimum value of t for this curve is $9\kappa^2$.

For the third term in (116) to contribute, the necessary condition is

$$K(s, t; 4\kappa^2, 4\kappa^2) \neq 0$$

and the corresponding curve C_3 is given by

$$s(t - 16\kappa^2) - 16\kappa^4 = 0 \qquad (121)$$

As s becomes very large, this curve also asymptotically tends to a straight line and the minimum value of t is now $16\kappa^2$.

We therefore see that $\rho(s, t)$ vanishes uniformly for all values of s and t lying below the curve C_1. For this reason, one can replace the lower limit $4\kappa^2$ by 0 in the integrals occurring in equation (116).

Incidentally, we know that for physical cases $(1 - t/2s)$ must lie between -1 and $+1$, and in this region $t < 4\kappa^2$. Since ρ is zero in this region, we have the strange but inconsequential result that the Mandelstam representation can be calculated from ρ belonging to unphysical regions only.

Let us now calculate $\rho(s, t)$ explicitly for any real and positive s and t. We have already seen that for the region below C_1, ρ is uniformly zero. For the region between C_1 and C_2 we can calculate ρ exactly from the first term in (116). This turns out to be:

$$\rho(s,t) = \lambda^2 \frac{\pi}{2} \frac{1}{\left[s(t-4\kappa^2)t - t\kappa^4\right]^{1/2}} \qquad (122)$$

Above C_2 the second term also has to be taken into account. We can do this by substituting equation (122) into the integral, since $\rho(s', t')$ is known exactly for a certain region as discussed above. As long as the s' and t' values describe a point below C_2, we can compute the integral exactly, and $\rho(s, t)$ is also known exactly. This means that for any given value of $s' = s_o$, t' must be always less than t_m such that (s_o, t_m) lie on C_2. We can determine as a function of s_o from (120):

$$s_o (t_m - 9\kappa^2)(t_m - \kappa^2) - 4\kappa^2 t_m = 0 . \quad (123)$$

We next have to find for what region of the $s - t$ plane this procedure gives the exact $\rho(s, t)$. The θ-function appearing in the term under discussion is

$$\theta\left[t - t' - \kappa^2 - \frac{t'\kappa^2}{2s} - \frac{\sqrt{t'\kappa^2}}{2s}\left\{16s^2 + 4s(t' + \kappa^2) + t'\kappa^2\right\}^{1/2}\right]$$

It can be seen that for a fixed t there is a maximum value of t' for which the argument of the θ-function is positive. When $t' = t_m$, the argument will be zero for a certain t_D and s_D such that

$$t_D - t_m - \kappa^2 - \frac{t_m\kappa^2}{2s_D} - \frac{\sqrt{t_m\kappa^2}}{2s_D}\left\{16s_D^2 + 4s_D(t_m + \kappa^2) + t_m\kappa^2\right\}^{1/2}$$

(124)

Equation (124) with s_D and t_D as the variables will define a curve D in the $s - t$ plane.

Below this curve $\rho(s, t)$ ought to be calculated exactly from the first two terms alone, since when performing the integration over t' the kernel $K(s, t; t', \kappa^2)$ will be non-zero for those values of $\rho(s', t')$ which are already known.

However, D can be shown to lie above C_3 and therefore the above procedure gives an exact $\rho(s, t)$ only below C_3.

To compute $\rho(s, t)$ above C_3 we adopt a similar technique. Since we know the weight function exactly upto C_3 we can substitute it in the third term and find ρ exactly upto another curve above C_3. In this manner, we can cover the entire $s - t$ plane, if necessary. Otherwise, we can compute ρ exactly only upto some required region. The essential point is that we have now developed a technique for finding ρ to arbitrary accuracy.

In the region between C_1 and C_2 the weight function contains a factor λ^2. Beyond that it acquires terms containing higher powers of λ. Ultimately, $\rho(s, t)$ becomes a series in λ. If we actually stop the calculation of ρ at some region, the function will be only a polynomial in λ. This has some unique advantages over the Born series. First, the question of convergence does not arise since ρ is represented by a sequence of polynomials. Secondly we can find ρ and hence $f(s, t)$ upto a certain power of λ and this

value will be an exact value. Thus the uncertainty in the Born approximation is avoided.

We have thus found ρ but only in the case when there are no bound states and no subtraction terms. If bound states occur, we shall only have extra terms and the curves C_1 etc. will be modified. The calculation will be more tedious, but possible. But if subtraction terms are present, then the q_j's also have to be calculated, and the resulting set of non-linear integral equations become extremely complicated. These complications are removed to a large extent by studying the Mandelstam representation in terms of partial waves. This representation is generally found more useful.

Chapter V.

DISPERSION RELATIONS FOR PARTIAL WAVE AMPLITUDES

It is well known that the total scattering amplitude can be expanded in a series of partial waves,

$$f(s,t) = \frac{1}{\sqrt{s}} \sum_{\ell=0}^{\infty} (2\ell+1)\, e^{i\delta_\ell(s)} \sin\delta_\ell(s)\, P_\ell\left(1 - t/2s\right) \tag{125}$$

s and t are real.

Defining

$$f_\ell(s) = \frac{1}{\sqrt{s}}\, e^{i\delta_\ell(s)} \sin\delta_\ell(s) \tag{126}$$

as the partial wave amplitudes, we have

$$f(s,t) = \sum_{\ell=0}^{\infty} (2\ell+1)\, f_\ell(s)\, P_\ell\left(1 - t/2s\right) \tag{127}$$

We can invert the above equation with the aid of the orthonormal property of the Legendre polynomials and write

$$f_\ell(s) = \frac{1}{2} \int_{-1}^{+1} f(s,x)\, P_\ell(x)\, dx \tag{128}$$

with $x = 1 - t/2s$.

Our aim here is to obtain dispersion relations for the partial wave amplitudes. Let us assume one S-wave bound state, and assume that only one subtraction is needed. We have the Mandelstam representation as

$$f(s,t) = f_B(t) + \frac{R}{s+|\epsilon|} - \lim_{\eta\to 0} \frac{t}{\pi^2} \int_0^\infty\!\!\int_0^\infty \frac{\rho(s',t')\, dt'\, ds'}{(t'+t)\, t'\, (s'-s-i\eta)}$$

$$+ \lim_{\eta\to 0} \frac{1}{\pi} \int_0^\infty \frac{g(s')}{s'-s-i\eta}\, ds' \tag{129}$$

where $g(s) = \mathrm{Im}\ f(s,0)$. R is independent of t since the highest power of t in $R(|\epsilon|, t)$ is $\ell = 0$. For Yukawa potential it is easily shown that

$$f_B = -\frac{\lambda}{t+\kappa^2} \tag{130}$$

The next step consists in substituting equation (129) in (128). The Born term will then yield the integral

$$\frac{1}{2}\int_{-1}^{+1} \frac{P_\ell(x)\,dx}{\kappa^2 + 2s(1-x)}$$

The third term in (129) will contain the integral

$$\frac{1}{2}\int_{-1}^{+1} \frac{P_\ell(x)\,dx}{t' + 2s(1-x)}$$

In general we have to deal with the integral

$$\bar{I}_\ell = \frac{1}{2}\int_{-1}^{+1} \frac{P_\ell(x)\,dx}{a + 2s(1-x)} \tag{131}$$

where a stands for κ^2, t.

We now need some properties of the Legendre functions of the second kind defined by

$$Q_\ell(y) = \frac{1}{2}\int_{-1}^{+1} \frac{P_\ell(x)}{y-x}\,dx \tag{132}$$

In particular, we have

$$\begin{aligned} Q_0(y) &= \frac{1}{2}\log\frac{y+1}{y-1} \\ Q_1(y) &= -1 + \frac{1}{2}\log\frac{y+1}{y-1} \end{aligned} \tag{133}$$

From the definition of $Q_\ell(y)$ given above, we can deduce the recurrence relation

$$Q_{\ell+1}(y) = \frac{2\ell+1}{\ell+1}\,y\,Q_\ell(y) - \frac{\ell}{\ell+1}\,Q_{\ell-1}(y)\ ;\ \ell > 1 \tag{134}$$

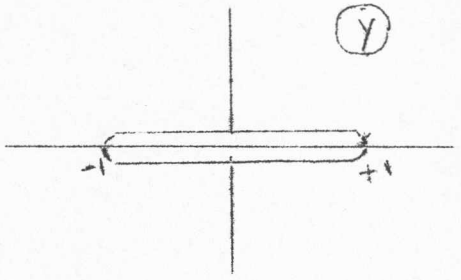
using which, higher $Q_\ell(y)$ may be determined. Also $Q_\ell(y)$ is real for $|y| > 1$ and complex for $|y| < 1$. To analytically continue the Q function to complex values of y, we make use of Schwartz's reflection principle,

$$Q_\ell^*(z) = Q_\ell(z^*)$$

It is to be noted from the definition of $Q_\ell(y)$ [cf. equation (132)] that $Q_\ell(y)$ has branch points at $y = 1$ and $y = -1$. For convenience the branch cut connecting these points is laid along the real axis. Using the integral definition of $Q_\ell(y)$ and the relation $\lim_{\eta \to 0} \frac{\eta}{(y-x)^2+\eta^2} = \pi \delta(y-x)$ we can prove that the discontinuity along the cut is

$$D_\ell(y) = \frac{1}{2i} \lim_{\eta \to 0} \left[Q_\ell(y+i\eta) - Q_\ell(y-i\eta) \right]$$

$$= -\frac{\pi}{2} P_\ell(y) \; ; \qquad |y| < 1$$



With the aid of Schwartz's reflection principle we can prove that the discontinuity gives $\mathrm{Im}\, Q_\ell$. Comparing equation (131) and equation (132), we immediately write down

$$I_\ell(s) = \frac{1}{2s} Q_\ell\left(\frac{a}{2s} + 1\right), \quad a > 0 \qquad (135)$$

It is obvious that,

$I_\ell(s)$ is real for $s > -a/4$

and complex for $s < -a/4$

The branch points of I_ℓ occur at $s = -a/4$ and $s = -\infty$. The discontinuity along the cut is given by

$$\frac{1}{2i} \lim_{\eta \to 0} \left[I_\ell (s+i\eta) - I_\ell (s-i\eta) \right]$$

$$= \frac{1}{2s} \frac{\pi}{2} P_\ell (1 + a/2s) \quad ; s < -a/4 \qquad (136)$$

This discontinuity gives $\mathrm{Im} \frac{1}{2s} Q_\ell (1 + a/2s)$

Now we resume the discussion on the partial wave dispersion relations. Substituting (129) into (128) we arrive at the relation, for $\ell = 0$,

$$f_0(s) = -\frac{\lambda}{2s} Q_0 \left(1 + \frac{\kappa^2}{2s}\right) + \frac{R}{s + |\epsilon|}$$

$$+ \frac{1}{\pi^2} \lim_{\eta \to 0} \int_0^\infty \int_{4\kappa^2}^\infty \frac{\rho(s',t')}{s'-s-i\eta} \frac{1}{2s} \left[Q_0 (1 + t'/2s) - \frac{2s}{t'} \right] dt' ds'$$

$$+ \frac{1}{\pi} \lim_{\eta \to 0} \int_0^\infty \frac{q(s')}{s'-s-i\eta} ds' \qquad (137)$$

and for any $\ell \geq 1$

$$f_\ell (s) = -\frac{\lambda}{2s} Q_\ell \left(1 + \frac{\kappa^2}{2s}\right) + \frac{1}{\pi^2} \lim_{\eta \to 0} \int_0^\infty \int_{4\kappa^2}^\infty \frac{\rho(s',t')}{s'-s-i\eta} \frac{1}{2s} Q_\ell \left(1 + \frac{t'}{2s}\right) d$$

(138)

This set of equations is called the Mandelstam representation for the partial wave amplitudes. In (138) we find that the integral $\frac{1}{\pi} \int_0^\infty \frac{q(s')}{s'-s-i\eta}$ is absent. This is due to the fact

$$\int_{-1}^{+1} P_\ell (x) dx = \frac{2}{2\ell+1} \delta_{o\ell}$$

Thus to obtain $f_\ell(s)$, $\ell \geq 1$ we note that we have to merely evaluate the integral after substituting for $\rho(s',t')$. Taking the imaginary part of (137) and rearranging,

$$g(s) = \mathrm{Im}\, f_0(s) - \frac{1}{\pi}\int_{4\kappa^2}^{\infty} \rho(s,t')\,\frac{1}{2s}\left[Q_0\left(1+\frac{t'}{2s}\right) - \frac{2s}{t'}\right] dt' \qquad (139)$$

Thus, on the other hand, when substituting for $g(s)$ in (137) we arrive at a non-linear integral equation for f_0. The non-linearity enters through the unitarity condition for partial wave amplitudes

$$\mathrm{Im}\ f_\ell(s) = \sqrt{s}\,|f_\ell(s)|^2 \qquad (140)$$

The '' N/D method'' by which the integral equation (138) is solved is indicated later.

Analytic Properties of Partial Wave Amplitudes:

We can study the analytic properties of partial wave amplitudes from the Mandelstam representations (137) and (138), for all ℓ including $\ell = 0$. The amplitudes $f_\ell(s)$ have a cut from $s = 0$ to $s = +\infty$ along the real axis. This cut arises from the denominator $s - s'$. It may be recalled that the full amplitude $f(s,t)$ also had a similar behaviour. In the present case, there is also a cut on the negative real axis. The Born terms have a cut starting from $s = -\frac{\kappa^2}{4}$ to $s = -\infty$. This cut arises from the behaviour of the Q functions. Also the double integral terms possess a cut from $s = -\kappa^2$ (this is because the lower limit for t' is $4\kappa^2$) to $s = -\infty$. Another obvious property in the case of $f_0(s)$ is that it has

a pole at $s = -|\xi|$. This however does exhaust all the singularities of the partial wave amplitudes. We have shown earlier (cf. strip approximation) that the successive approximation of the integral equation for ρ amounts essentially to a series expansion of ρ as

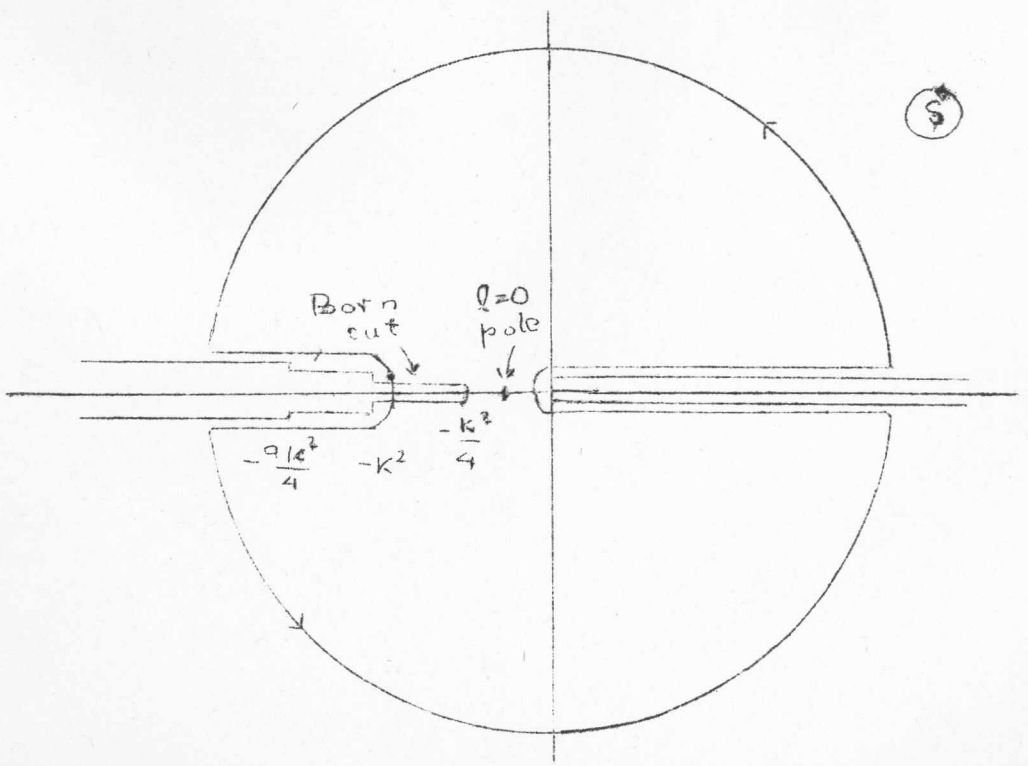
$$\rho(s',t') = \rho^{(1)} + \rho^{(2)} + \rho^{(3)} + \cdots \quad (141)$$

where

(1) the successive terms of the series contain powers of λ, the strength parameter, starting from λ^2, and

(2) $\rho^{(n)}$ vanishes unless $t' \geq (n+1)^2 K^2$. Therefore, for the $n'th$ term the effective lower limit of integration in t' is $(n+1)^2 K^2$. Hence branch points are situated at the corresponding values of $-\frac{(n+1)^2 K^2}{4}$ i.e. at

$$s = -K^2, \; -\frac{9}{4}K^2, \; -\frac{16}{4}K^2, \; \cdots$$



Thus there is an overlapping of the associated branch cuts. This is the reason why the branch points other than $-\frac{\kappa^2}{4}$ were not obvious at first. However, if the Born term is discarded, the cut starts at $-\kappa^2$. It is to be noted that the relative positions of the branch points are maintained for all ℓ, but the actual discontinuities vary with ℓ.

Explicit Partial Wave Dispersion Relations:

It is useful to reformulate the dispersion relations equation (137) and equation (138) in such a way as to bring out the analytic properties in them explicitely. We adopt the customary technique of invoking Cauchy's theorem. To this end we choose the contour shown in the figure above. Also we must know the asymptotic behaviour of $f_\ell(s)$. The unitarity condition is

$$\mathrm{Im}\ f_\ell(s) = \sqrt{s}\ |f_\ell(s)|^2$$

Along the real axis, we can show that

$$|f_\ell(s)|^2 < \frac{1}{\sqrt{s}} \qquad (142)$$

Therefore $f_\ell(s) \to 0$ as $|s| \to \infty$. We can analytically extend the unitarity relation to complex values of s and prove that $f_\ell(s) \to 0$ in any direction. To allow for the real values of s on the cut we can slightly displace the cut below the real axis and take the limit as the cut tends to align itself along the real axis. Applying Cauchy's theorem to $(f_\ell - f_{\ell B})$ we write down the following equations for $f_\ell(s)$ whose analytic properties are compatible with those discussed above:

$$f_0(s) = f_{0B}(s) + \frac{R}{s+|\epsilon|} + \int_0^{\infty} \frac{A_0(s')}{s'-s-i\eta}\, ds' + \int_{-\infty}^{-\kappa^2} \frac{B_0(s')}{s'-s-i\eta}\, ds' \qquad (143)$$

$$f_\ell(s) = f_{\ell B}(s) + \int_0^{\infty} \frac{A_\ell(s')}{s'-s-i\eta}\, ds' + \int_{-\infty}^{-\kappa^2} \frac{B_\ell(s')}{s'-s-i\eta}\, ds'$$

Here $f_{\ell B}(s)$ stands for $-\frac{\lambda}{2s} Q_\ell\left(1+\frac{\kappa^2}{2s}\right)$. The meaning of $A_\ell(s')$ and $B_\ell(s')$ becomes clear if we consider the imaginary part of equations (143). When $s > 0$,

$$\mathrm{Im}\, f_\ell(s) = \pi A_\ell(s) \qquad (144a)$$

The second integral of (143) will not contribute since the argument of the δ function is outside the range of integration. Similarly, when $s < -\kappa^2$

$$\mathrm{Im}\left[f_\ell(s) - f_{\ell B}(s)\right] = \pi B_\ell(s) \qquad (144b)$$

As before, no contribution comes from the first integral because the argument to the δ function is beyond the limits of integration. Therefore we arrive at the explicit form of the partial wave dispersion relations

$$f_0(s) = f_{0B}(s) + \frac{R}{s+|\epsilon|} + \frac{1}{\pi}\int_0^{\infty} \frac{\mathrm{Im} f_0(s')}{s'-s-i\eta}\, ds' + \frac{1}{\pi}\int_{-\infty}^{-\kappa^2} \frac{\mathrm{Im}\left[f_0(s') - f_{0B}(s')\right]}{s'-s-i\eta}\, ds'$$

$$f_\ell(s) = f_{\ell B}(s) + \frac{1}{\pi}\int_0^\infty \frac{\mathrm{Im}\, f_\ell(s')}{s'-s-i\eta}\,ds' + \frac{1}{\pi}\int_{-\infty}^{-\kappa^2} \frac{\mathrm{Im}\left[f_\ell(s') - f_{\ell B}(s')\right]}{s'-s-i\eta}\,ds' \qquad (145)$$

In the latter equation, that is, for $\ell \geq 1$ the integrands can be determined explicitly from the original dispersion relation (138). For the range $0 < s < \infty$, the Born term is real, and so if we take the imaginary part of both sides of equation (133) we have

$$\mathrm{Im}\, f_\ell(s) = \frac{1}{2\pi s}\int_{4\kappa^2}^\infty \rho(s,t')\, Q_\ell\left(1+\tfrac{t'}{2s}\right)dt', \qquad (0<s<\infty) \qquad (146a)$$

For the range $-\infty < s < -\kappa^2$, the Born term is complex and makes a contribution, but now the term in η on the right of (138) is of no consequence. Hence, taking imaginary parts, and using (136):

$$\mathrm{Im}\left[f_\ell(s) - f_{\ell B}(s)\right] = \frac{1}{4\pi s}\int_0^\infty\int_{4\kappa^2}^\infty \frac{\rho(s',t')}{s'-s}\, P_\ell\left(1+\tfrac{t'}{2s}\right) \theta\left(-s-\tfrac{t'}{4}\right) dt'\,ds', \qquad (-\infty<s<-\kappa^2) \qquad (146b)$$

The right hand sides of equations (146) are completely known functions. They can be used in equation (145) to evaluate $f_\ell(s)$ for $\ell \neq 0$. It is therefore clear that no integral equations are involved, and that only ordinary integrations have to be performed.

However, the situation is different for the case $\ell = 0$. An unknown function $g(s)$ is present. Moreover, the non-linear nature of the integral equation for $f_0(s)$ is made evident

on substituting

$$\mathrm{Im}\ f_0(s) = \sqrt{s}\ |f_0(s)|^2$$

in the first of the equations (145).

The N/D Method.

In the previous section it was shown that for $\ell = 0$ we have to solve a nonlinear integral equation in $f_0(s)$. To accomplish this Noyes and Wong* proposed a method known as "the N over D method".

Let us try the representation

$$f_0(s) = \frac{N(s)}{D(s)} \qquad (147)$$

The following assumptions are made about the analytic behaviour of $N(s)$ and $D(s)$.

(1) N is real for $s > 0$, and has a branch cut along the negative real axis from $s = -\frac{\kappa^2}{4}$ to $s = -\infty$.

and (2) D is real for $s < 0$, and has a branch cut along the positive real axis from $s = 0$ to $s = \infty$.

Neither N nor D has any other singularity than the above mentioned cuts. The following assumptions are made about the asymptotic behaviour of N and D:

(1) $D(s) \to +1$ when $|s| \to \infty$.

and (2) $N(s) \to 0$ when $|s| \to \infty$.

These properties of N and D agree with the analytic behaviour of $f_0(s)$. The choice of the ratio of $N(s)$ and $D(s)$ leads to integral equations separately for N and D. The N/D method emphasizes the fact that $f_0(s)$ is completely

* P. Noyes--D.Y.Wong, Phys. Rev. Letters 3, 191 (1959).

determined purely by its singularities and the unitarity condition.

Making use of Cauchy's integral theorem we arrive at the following integral representations of $N(s)$ and $D(s)$:

$$N(s) = \frac{1}{\pi} \int_{-\infty}^{-K^2/4} \frac{\mathrm{Im}\ N(s')}{s' - s - i\eta}\, ds' \tag{148a}$$

$$D(s) = 1 + \frac{1}{\pi} \int_{0}^{\infty} \frac{\mathrm{Im}\ D(s')}{s' - s - i\eta}\, ds' \tag{148b}$$

Here we have two nonsingular integral equations of the Fredholm type. Since $N(s)$ is real for $s > 0$, we have

$$\mathrm{Im}\ D(s) = N(s)\ \mathrm{Im}\left[1/f_0(s) \right] \tag{149}$$

From the unitarity relation we obtain

$$\mathrm{Im}\left[1/f_0(s) \right] = \mathrm{Im}\ \frac{f_0^*}{|f_0|^2} = -\frac{1}{|f_0|^2}\, \mathrm{Im}\, f_0 = -\sqrt{s} \tag{150}$$

Substitution equation (150) in (149) we obtain

$$\mathrm{Im}\ D(s) = -\sqrt{s}\ N(s) \tag{151}$$

Therefore we can rewrite (148b) as

$$D(s) = 1 - \frac{1}{\pi} \int_{0}^{\infty} \frac{\sqrt{s'}\ N(s')}{s' - s - i\eta}\, ds' \tag{152}$$

We now use the fact that in the region $-\infty < s < -K^2/4$. $D(s)$ is real. Therefore

$$\mathrm{Im}\ N(s) = D(s)\ \mathrm{Im}\ f_0(s) \quad , \quad -\infty < s < -\frac{K^2}{4} \tag{153}$$

We have already seen that

$$\mathrm{Im}\, f_0(s) = \mathrm{Im}\, f_{0B}(s) + \frac{1}{4\pi s} \int_{0}^{\infty} \int_{4K^2}^{\infty} \frac{\rho(s', t')}{s' - s}\, P_0(1 + t'/2s)\, \Theta(-s - t'/4)\, dt'\, ds',$$

$$(-\infty < s < -K^2)$$

which gives $\mathrm{Im}\, f_{o}(s)$ in terms of ρ . Also it can be shown using the definition of f_{oB} that

$$\mathrm{Im}\, f_{oB} = -\frac{\lambda\pi}{4s}, \quad s < -\frac{K^2}{4} \tag{154}$$

Let us denote

$$\alpha(s) = \frac{\pi}{s}\left[-\lambda + \frac{1}{\pi^2}\int_0^\infty \int_{4K^2}^\infty \frac{\rho(s't')}{s'-s}\,\theta(-s-t'/4)\,dt'ds'\right] \tag{155}$$

Then

$$\mathrm{Im}\, N(s) = D(s)\,\alpha(s), \quad s < -\frac{K^2}{4} \tag{156}$$

Substituting equation (156) in equation (148a) , we obtain

$$N(s) = \frac{1}{\pi}\int_{-\infty}^{-K^2/4} \frac{D(s'')\,\alpha(s'')}{s''-s-i\eta}\,ds'' \tag{157}$$

Thus the expressions (152) and (157) together constitute a coupled integral equation. In these two equations we choose to eliminate N (s) . An elementary integration * over s' and proper substitution leads to the following expression for D (- s):

$$D(-s) = 1 + \frac{1}{\pi}\int_{K^2/4}^{\infty} \frac{\alpha(-s'')\,D(-s'')}{\sqrt{s''}+\sqrt{s}}\,ds'' \tag{158}$$

This is a singular Fredholm type integral equation. To convert equation (158) into a non-singular Fredholm type integral equation we make the substitutions

$$y = \frac{1}{\sqrt{s}}$$
$$x^2 = \frac{1}{s''} \tag{159}$$

---

* Use has been made of the formula

$$\int_0^\infty \frac{\sqrt{s'}}{(s'-s)(s''-s')}\,ds' = -\frac{\pi}{\sqrt{s''}+\sqrt{s}}$$

to obtain

$$D(-y) = 1 + \frac{2}{\pi} \int_0^{2/K} \frac{1}{x^2} \frac{\alpha\left(-\frac{1}{x^2}\right)}{1 + \frac{x}{y}} D(-x)\, dx \qquad (160)$$

Equation (160) can be solved by employing any one of the standard methods. Then to get $N(s)$ is merely a matter of substitution of D thus obtained in equation (157) and the evaluation of the corresponding quadrature. Knowing N and D, $f_o(s)$ is directly given. However the exact solution of (160) is difficult to obtain. So we are likely to encounter difficulties. The representation $f_o = N / D$ holds true in the case of potential scattering (cf. Jost functions); but in Field Theory the proof of such a representation gives rise to serious difficulties.

One advantage of the N/D method is that it gives quickly the bound state of the system under consideration since the poles of $f_o(s)$ which correspond to the bound states are simply the zeros of $D(s)$. That is, the solution of

$$1 + \frac{2}{\pi} \int_0^{2/K} \frac{\alpha\left(-\frac{1}{x^2}\right) D(-x)}{x^2 \left(1 + \frac{x}{y}\right)} dx \qquad (161)$$

enables us to calculate the binding energy of the system. Since the residue of $f_o(s)$ is the value of $N(s)$ at the pole $s = -|\varepsilon|$, we can also calculate the residue R.

The Pole Approximation:

Chew and Mandelstam have suggested that the contribution from the left hand cut can be approximately replaced by that from a pole. This is analogous to replacing a line charge by a point charge. The procedure, though mathematically unsound, yields solutions to a reasonable accuracy. Strictly speaking, the

approximation is valid for values $s > 0$ upto some s_{max} such that s_{max} is short compared with the "average" distance between the important left-hand singularities. $Im\, f_0(s)$ is a function of s along the negative real s-axis. But by replacing the cut by a pole we make it equal to zero everywhere except at $s = -s_0$ $(s_0 > 0)$., i.e., we set

$$Im\, f_0(s) = -\pi F\, \delta(s + s_0) \quad ; \quad s < -\frac{k^2}{4} \tag{162}$$

Here F characterizes the strength of the pole (figuratively the amount of line charge concentrated). As

$$\begin{aligned} Im\, N(s) &= D(s)\, Im\, f_0(s) \quad , \qquad s < -\frac{k^2}{4} \text{ we get} \\ Im\, N(s') &= D(s')\, Im\, f_0(s') \\ &= -\pi F\, D(s')\, \delta(s' + s) \end{aligned} \tag{163}$$

Substituting equation (163) in (148a) we arrive at

$$N(s) = F\, \frac{D(-s_0)}{s_0 + s} \tag{164}$$

Substituting this in the equation for D (equation 152), we get

$$\begin{aligned} D(s) &= 1 - \frac{F\, D(-s_0)}{\pi} \int_0^\infty \frac{\sqrt{s'}\, ds'}{(s' - s - \eta)(s_0 + s')} \\ &= 1 - F\, \frac{D(-s_0)}{\sqrt{s_0} + \sqrt{-s}} \end{aligned} \tag{165}$$

Assuming that this is valid for every s, we put $s = -s_0$. After rearrangement we get

$$D(-s_0) = \frac{2\sqrt{s_0}}{F + 2\sqrt{s_0}} \tag{166}$$

We have so far been concerned with the evaluation of quadratures,

and no integral equation was involved. Again, substituting for $D(-s_0)$ from equation (166) in equations (164) and (165), we obtain

$$N(s) = \frac{2F\sqrt{s_0}}{(F+2\sqrt{s_0})(s_0+s)} \tag{167a}$$

$$D(s) = 1 - \frac{2F\sqrt{s_0}}{(F+2\sqrt{s_0})(\sqrt{s_0}+\sqrt{-s})} \tag{167b}$$

Using $f_0 = N / D$ we get

$$f_0(s) = \frac{2F\sqrt{s_0}}{(s+s_0)} \quad \frac{(\sqrt{s_0}+\sqrt{-s})}{(F+2\sqrt{s_0})(\sqrt{s_0}+\sqrt{-s}) - 2F\sqrt{s_0}} \tag{168}$$

We note here that there is a pole at $s = -s_0$. However this formula is not valid on the cut from $-\frac{\kappa^2}{4}$ to $-\infty$.

To check the range of validity of this solution and to get at the physical meaning of the input parameters F and s_0, we shall compare our results with the effective range formula

$$\sqrt{s}\cot\delta_0(s) = -\frac{1}{\alpha} + \frac{1}{2}r_{eff}\,s \quad , s>0 \tag{169}$$

where $\delta_0(s)$ is the S-wave phase-shift, r_{eff}, the effective range of the scattering potential and α, the scattering length. From the definition of $f_0(s)$

$$\sqrt{s}\,\frac{R_e f_0(s)}{q_m f_0(s)} = \sqrt{s}\cot\delta_0 \tag{170}$$

For $s > 0$, we get from equation (168)

$$\sqrt{s}\cot\delta_0 = \frac{F+2\sqrt{s_0}}{2Fs_0}\left(\frac{2\sqrt{s_0}-F}{2\sqrt{s_0}+F}\,s_0 + s\right) \tag{171}$$

Here $\sqrt{s}\cot\delta_0$ is given in terms of the parameters F and s_0

and the variable s. Thus the pole approximation is in fact equivalent to the effective range approximation. Now it is possible to express the phenomenological parameters F and s_0 in terms of α and r_{eff} by comparing equations (169) and (171),

$$1/\alpha = -(1/F)\, s_0 + \tfrac{1}{2}\sqrt{s_0} \qquad (172a)$$

$$r_{eff} = 2/F + 1/\sqrt{s_0} \qquad (172b)$$

Thus the range of validity of the pole approximation is the same as that of the effective range formula. The scattering length α can be easily calculated from low energy experiments on σ where $\sigma \simeq 4\pi |\alpha|^2$. α is real for elastic scattering and complex for inelastic scattering. We can compute r_{eff} if we know the approximate solution of the radial Schrodinger equation for low energy. Thus knowing α and r_{eff} we can calculage F and s_0 using equations (172a) and (172b).

We have mentioned earlier that bound states are given by the zeros of $D(s)$. Equating (167b) to zero and solving for $\sqrt{-s}$

$$\sqrt{-s} = \sqrt{s_0}\, \frac{F - 2\sqrt{s_0}}{F + 2\sqrt{s_0}} \qquad (173)$$

$\sqrt{-s}$ must be positive since, for a real bound state the pole must be on the first Riemann sheet. This in turn demands that $F \geq 2\sqrt{s_0}$ provided $F > 0$. Under these circumstances we see from equation (172a) that $\alpha > 0$. In fact this is the condition for the existence of a bound state. If $F < 0$, α is

+ve or -ve according as $|F| >$ or $< 2\sqrt{s_0}$. But it is clear from equation (173) that for $\sqrt{-s}$ to be positive, $|F| > 2\sqrt{s_0}$. Here it is to be noted that the pole approximation is valid for low energy only.

To improve the accuracy of the approximation, the left hand cut can be replaced by more than one pole. But this procedure brings in its wake new input parameters.

Remarks on the case of several bound states:

If there are $(N+1)$ subtractions in the full Mandelstam representation, then $f_\ell(s)/s^n \to 0$ as $|s| \to \infty$, that is, there will be at most n subtractions needed for each f_ℓ. Apart from this, in the case of partial waves with $\ell \geq n+1$ we have to evaluate quadratures over the ρ's which are known in principle. If $\ell < n+1$ we encounter non-linear integral equations. These can be reduced to non-singular Fredholm type equations by using the ansatz $f_\ell = N_\ell / D_\ell$. The kernel of these integral equations will be given in terms of the weight functions ρ, but subtracted dispersion relations may now be needed for the N equations. The subtraction constants $N_\ell(s)$ however remain undetermined. It appears that the Mandelstam representation coupled with unitarity may form the basis of a complete dynamical scheme, entirely replacing the conventional Schrodinger equation approach, both for the scattering problem and for the bound state problem. The interaction is characterized by its range and strength. These characteristics control the analytic behaviour of f. From the analytic properties all partial wave amplitudes can be determined. The poles of the

amplitudes can then be interpreted as bound states. There is, however, one snag. The exact number of subtractions in the full amplitude is not known. Even if we make a good guess we are still in the dark about the parameters. There are, however, two ways out of this difficulty, viz.,

(1) to employ a Perturbational approach;

and (2) study ''further'' analytic properties of $f_Q(s)$.

The latter approach, developed by Regge may give sufficient information which elucidates the exact number of subtractions.

Chapter VI.

THE REGGE POLES.

Regge's * starting point is trivial both mathematically and physically. His approach essentially consists in 'complexifying' the angular momentum ℓ in $f_\ell(s)$,

$$f_\ell(s) \longrightarrow f(\ell, s)$$

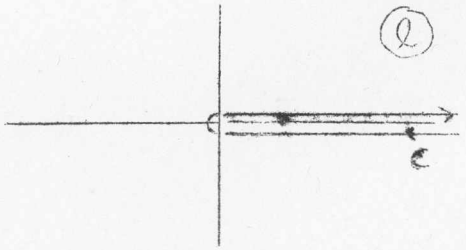
where ℓ is complex and continuous. The partial wave decomposition of the scattering amplitude is performed as usual:

$$f(s, z) = \sum_{\ell=0}^{\infty} (2\ell+1)\, f(\ell, s)\, P_\ell(z) \qquad (174)$$

where $z \equiv \cos\vartheta$ and $f(\ell, s) = \frac{1}{\sqrt{s}} e^{i\delta_\ell(s)} \sin\delta_\ell(s)$. At this stage ℓ is real and positive. As our aim is to treat ℓ as a continuous complex variable, the problem immediately on hand is to replace the summation by an integration. A well known mathematical theorem by Sommerfeld and Watson enables us to do this. According to this theorem

$$f(s, z) = -\frac{i}{2} \int_C \frac{2\ell+1}{\sin\pi\ell}\, f(\ell, s)\, P_\ell(-z)\, d\ell \qquad (175)$$

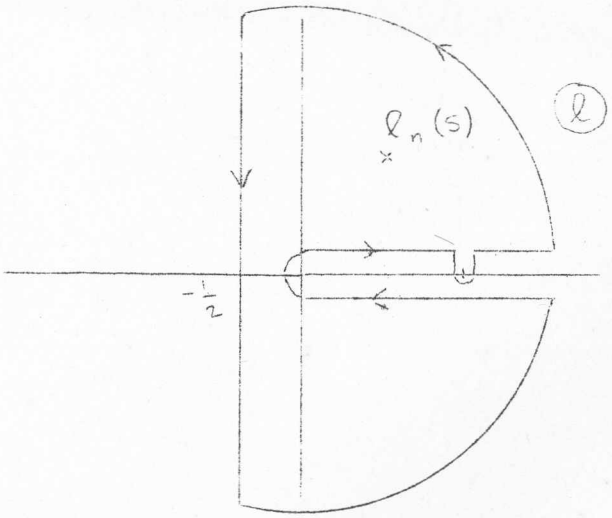
where the contour C surrounds the real positive ℓ-axis as indicated in the figure.



* T. Regge, Nuovo Cimento 14, 951 (1959); ibid 18, 947 (1960); see also W. Kummer, CERN Report 62-14, March 1962.

If $f(\ell, s)$ has no accidental poles for ℓ real and positive, the poles of the integrand are situated at $\ell = 0, 1, 2 \ldots$ We can evaluate the contour integral (175) with the contour indicated in the figure and retrieve equation (174). If there are accidental poles, we can exclude them by an indentation of the contour.

Regge has shown from the study of the radial Schrodinger equation that $f(\ell, s)$ in the integrand of equation (175) has only a finite number of poles for $Re\ \ell > -1/2$ and that all complex poles lie in the upper half plane, $Im\ \ell \geq 0$. If we consider a continuous superposition of Yukawa potentials, then it can be shown that $f(\ell, s) \to 0$ when $\ell \to \infty$ faster than $P_\ell / \sin \pi\ell$. This asymptotic behaviour of the integrand enables us to use the contour indicated in the figure



The contribution from the large arcs is zero. Therefore

$$f(s, \xi) = \frac{i}{2} \int_{-\frac{1}{2}+i\infty}^{-\frac{1}{2}-i\infty} \frac{2\ell+1}{\sin \pi\ell} f(\ell, s) P_\ell(-\xi)\, d\ell + \sum_{n=1}^{N} \frac{\beta_n(s)}{\sin \pi \ell_n} P_{\ell_n}(-\xi) \qquad (176)$$

where ℓ_n is the n^{th} pole and β_n is given by

$$\beta_n = 2\pi i\, (2\ell_n + 1) \lim_{\ell \to \ell_n} \left[(\ell - \ell_n) f(\ell, s) \right] \qquad (177)$$

The poles ℓ_n are called the ''Regge Poles''; for $s < 0$, they correspond to bound states; for $s > 0$ they correspond to resonances as will be discussed below. Note in equation (176) that the singular parts of the amplitude are separated from the smooth integral form. It should be remembered that both the ℓ_n and β_n depend on the energy s.

For large ζ and $\mathrm{Re}\,\alpha > -1/2$,

$$P_\alpha(-\zeta) \approx \zeta^{\mathrm{Re}\,\alpha} \quad \ldots$$

So the integral term in equation (176) is the limit $|\zeta| \to \infty$ does not contribute, since $\mathrm{Re}\,\ell = -1/2$. Therefore for large ζ the behaviour of f is dominated by that Regge pole which has the largest $\mathrm{Re}\,\ell_n$. Let us denote this farthese pole by L,

$$f(s,t) \to t^{\mathrm{Re}\,\ell} \quad \text{for } |t| \to \infty \qquad (178)$$

There is only a finite number of Regge poles and therefore $\mathrm{Re}\,L$ is finite. So $f(s, t)$ behaves as a polynomial. As $f(s,t)$ has no essential singularities it is possible to write down a dispersion relation for $f(s, t)$ in t. (This was so far a tacit assumption !) Now it is also possible to calculate the exact number of subtractions to be performed to establish the Mandelstam representation. Writing

$$\mathrm{Re}\,L = \ell_i + \tau \qquad (179)$$

where ℓ_i is the smaller of the two integers nearest to $\mathrm{Re}\,L$, it follows that

$$\frac{f(s,t)}{t^{\ell_i+1}} \approx \frac{1}{t^{1-\tau}} \to 0 \quad \text{as } |t| \to \infty$$

Therefore $\ell_i + 1$ is the smallest power to which we have to raise t before dividing $f(s,t)$ to get the asymptotic

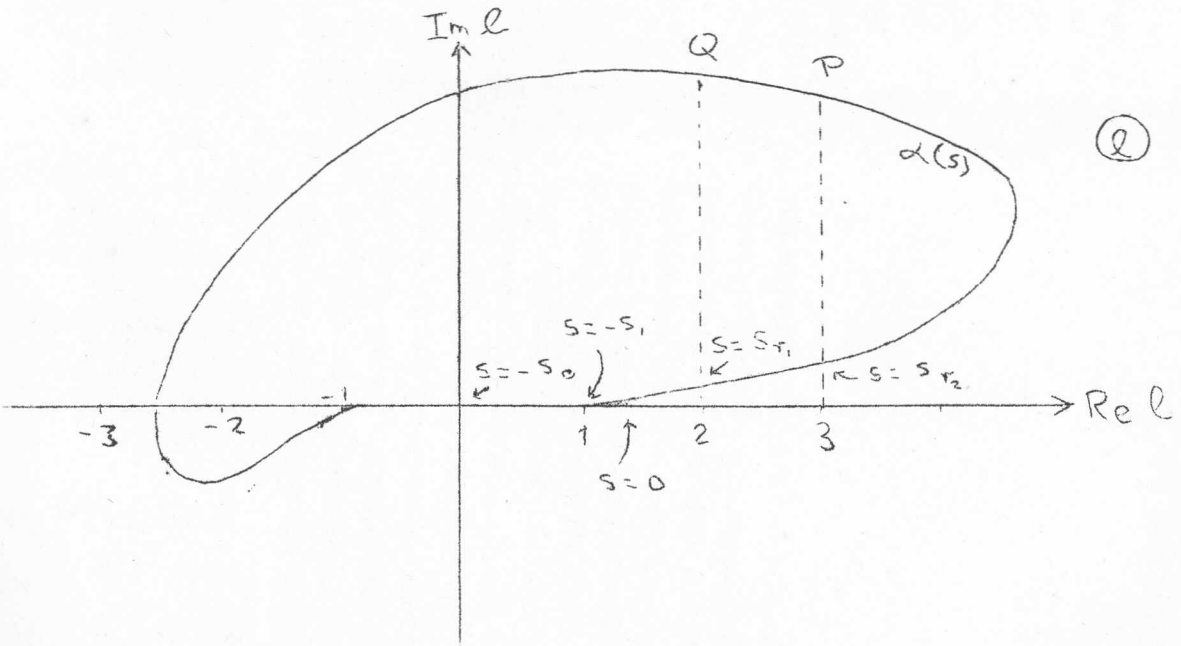
behaviour. Therefore the number of subtractions in the full Mandelstam representation is $\ell_i + 1$ where ℓ_i is the nearest integer defined by equation (179). This is an exact statement but we do not know yet the physical meaning of the farthest pole. We shall discuss the meaning of the Regge poles below.

Relation between Regge poles and Bound states and Resonances:

We have indicated that the ℓ_n's are energy dependent,

$$\ell_n = \alpha(s)$$

This equation describes the motion of the Regge pole ℓ_n. The following figure indicates a typical "Regge trajectory".



As long as the energy is negative ($s < 0$) the poles lie on the real axis. At $s = 0$ the trajectory leaves the real axis and goes upward. For a small imaginary part, $\mathrm{Re}\,\ell$ increases monotonically with respect to the energy s. For some values of $\ell\,(\mathrm{Re}\,\ell, \mathrm{Im}\,\ell)$ the slope of the trajectory is infinite. The curve then turns

back and completes the loop joining the negative real axis at some negative value as $s \to +\infty$. It may also happen that the curve cuts first the negative real axis at some negative half integral value.

In the vicinity of a bound state or a resonance the magnitude of the scattering amplitude is very large. From equation (176) it is clear that $|f(s, z)|$ is large near the poles. Therefore, we are led to identify the bound states and resonances with the Regge poles. Let the residue corresponding to $\ell_n = \alpha(s)$ be $\beta_n = \beta(s)$. We can arrive at an approximate expression for the total amplitude,

$$f(s, z) \approx \frac{\beta(s)}{\sin \pi \alpha(s)} \; P_{\alpha(s)}(-z) \qquad (180)$$

To get an approximate expression for $f_\ell(s)$ we must project the contribution to a specific partial wave. We know that

$$f_\ell(s) = \frac{1}{2} \int_{-1}^{+1} f(s, z) \, P_\ell(z) \, dz$$

where ℓ is a non-negative integer. It is known that generalising the orthogonality relation between the Legendre polynomials one gets

$$\frac{1}{2} \int_{-1}^{+1} P_\ell(z) \, P_\ell(-z) \, dz = \frac{1}{\pi} \frac{\sin \pi \alpha}{(\alpha - \ell)(\alpha + \ell + 1)} \qquad (181)$$

From (180) we then obtain

$$f(\ell, s) \approx \frac{1}{\pi} \frac{\beta(s)}{[\alpha(s) - \ell][\alpha(s) + \ell + 1]} \; ; \ell = 0, 1, 2, \cdots \qquad (182)$$

Considered as a function of s, $f_\ell(s)$ has a pole when $\alpha(s) = \ell$. But we know that a pole in $f_\ell(s)$ implies a bound state with angular momentum ℓ. Thus whenever $\alpha(s)$ is equal to an

t," he wrote to Marie. He returned to Barmen, but his lofty, roloul found the parental home and office work in the family firm

integer we get a bound state. A single Regge pole causes bound states in several angular momentum states whenever its trajectory passes through a non-negative integr value ℓ . The figure given above shows the trajectory of the Regge pole which causes an $\ell = 0$ bound state with energy $s = - s_0$, and an $\ell = 1$ bound state with energy $s = - s_1$. From equation (182) it is obvious that $\alpha(s) = -(\ell + 1)$ also gives rise to poles. These poles could occur provided the curve rejoins the negative realaxis at a point less than -1. These poles do not however correspond to a physical situation as they occur with negative ℓ values.

Regge's approach elucidates resonances also. For instance let us suppose that for $s > 0$, in the monotonically increasing part of the curve, there exists a pole $\alpha(s)$ with its real part very nearly equal to an integer, plus a small imaginary part. Let this correspond to $S = S_r$. Expanding in the neighbourhood of $S = S_r$:

$$\alpha(s) \approx \ell + \left(\frac{d}{ds} \mathrm{Re}\,\alpha\right)_{s=s_r} (s-s_r) + i\left(\mathrm{Im}\,\alpha\right)_{s=s_r}$$

Substituting for $\alpha(s)$ in equation (182) we get

$$f_\ell(s) \approx \frac{\beta(s)}{\left[2\ell+1 + i\left(\mathrm{Im}\,\alpha\right)_{s=s_r}\right]} \frac{1}{A\left[(s-s_r) + i\,\Gamma/2\right]} \qquad (183a)$$

where

$$A \equiv \left(\frac{d}{ds} \mathrm{Re}\,\alpha\right)_{s=s_r}$$

$$\frac{\Gamma}{2} \equiv \left(\mathrm{Im}\,\alpha\right)_{s=s_r} \Big/ \left(\frac{d}{ds} \mathrm{Re}\,\alpha\right)_{s=s_r} \qquad (183b)$$

If $\left(\mathrm{Im}\ \alpha\right)_{s=s_r}$ is negligible, $f_\ell(s)$ has a pole at $s = s_r$. This corresponds to a resonance with a half width $\Gamma/2$. Thus we have a resonance in the partial wave ℓ whenever the Regge trajectory, after leaving the real axis, comes close to a physical ℓ. If, after leaving the real axis, a Regge pole travels close to the real axis past several angular momentum states, then we have resonances in all those angular momentum states. In the diagram shown already, we have a D-resonance at $s = s_{r_1}$ and an F-resonance at $s = s_{r_2}$ which is weaker. It is to be noted that points like P and Q have a very large imaginary part and hence do not correspond to a physically interesting situation.

It appears now that there is a coupling between different partial waves through a resonance. But this could have been anticipated from the Mandelstam representation of the partial wave amplitudes where the same weight function ρ occurs in all the dispersion relations for different ℓ.

Now we are in a position to discuss the question of the number of subtractions to be performed in the Mandelstam representation. Let ℓ_{max} denote the bound state with the maximum angular momentum caused by a Regge pole and suppose that the trajectory turns back before $\mathrm{Re}\,\ell = \ell_{max} + 1$. We now recall that the large t behaviour of $f(s,t)$ will be dominated by that Regge pole which lies farthest to the right in the complex ℓ plane. If there is no other Regge trajectory which extends farther to the right then we can put, in the notation explained already, $\ell_i = \ell_{max}$. Thus we see that we need one

more subtraction above the angular momentum of the bound state with the maximum angular momentum. But if the same trajectory or any other trajectory possesses resonances with $\ell > \ell_{max}$ then the number of subtractions will be greater. Therefore it is only the minimum number subtractions that is determined by the bound states.

BEHAVIOUR OF HIGH ENERGY SCATTERING. *

The question to be discussed, very briefly, in this section is: Can Reggeology encompass relativistic elementary particles as well ? In potential scattering the high energy behaviour of the scattering amplitude and hence that of the differential scattering cross-section is known: $f(s) - f_{B} \to 0$ as $|s| \to \infty$. But in elementary particle theory the picture of a potential is of doubtful validity. To test whether the elementary particles do have a Regge behaviour, we observe the behaviour of σ_T at high energy.

The following are the salient experimental features of high energy scattering:

(1) The total-scattering cross-section tends to become energy independent for very high energies;

(2) At high energies the scattering is characterised by smooth variations with respect to energy; on the contrary there are numerous resonances found at low energy in strongly interacting systems;

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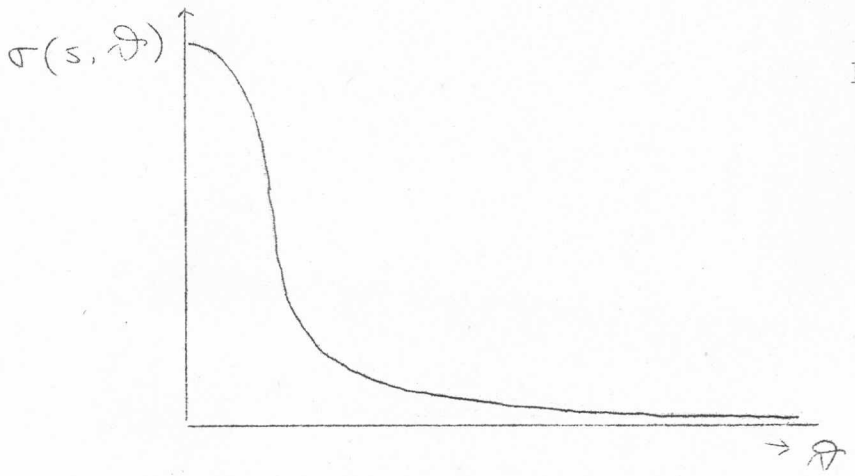
* For further details see: MATSCIENCE REPORT 8 - An Introduction to Complex Angular Momentum, Regge Poles and High Energy Scattering, by K. Raman.

(3) All elastic cross-sections show the characteristic diffraction pattern with a forward plane;

(4) At high energies, the elastic scattering amplitude is largely imaginary;

(5) At not too large energies the peripheral formulae seem to give the total cross sections well.



For s very high and fixed.

The above curve shows that the scattering tends to concentrate in the forward direction. An approximate expression for the total cross-section is obtained using the Born term:

$$\sigma_{total} = \int_{t=0}^{4s} |f_B(t,K)|^2 \, dt \qquad , (t = 2s(1-\cos\vartheta))$$

$$= \int \frac{dt}{(t+K^2)^2}$$

From this we can easily show that

$$\sigma_{total} \approx \frac{1}{K^2} \qquad \text{for} \quad s \to \infty . \qquad (184).$$

Expression (184) is verified at amazingly low energies for nucleon-nucleon scattering. For π N scattering the formula (184) is correct for much higher energies.

The variation of the width of the peak with energy s constitutes an interesting study. For high energies the width of the peak in the differential scattering cross-section is approximately the same as that of the diffraction peak. The angle corresponding to the half-width is given by

$$\sigma(s,\omega) = \frac{1}{2}\,\sigma(s,0) \tag{185}$$

But it is more convenient to deal with the scattering amplitude. So

$$f(s,\omega) = \frac{1}{2}\,f(s,0) \tag{186}$$

From equation (176),

$$f(s,\beta) = \frac{i}{2}\int_{-\frac{1}{2}+i\infty}^{-\frac{1}{2}-i\infty} \frac{2\ell+1}{\sin\pi\ell}\, f(\ell,s)\,P_\ell(-\beta)\,d\ell + \sum_{n=1}^{N} \frac{\beta_n(s)}{\sin\pi\alpha_n(s)}\,P_{\alpha_n}(s)(-\beta)$$

For very high energies the integral term does not contribute because of the presence of $\frac{1}{\sqrt{s}}$ term in $f(\ell,s)$. Also we make the assumption that only one of the N poles dominate, i.e., that pole for which β is highest and for which α is biggest for small values of β. These approximations lead to

$$f(s,\beta) \approx \frac{\beta(s)}{\sin\pi\alpha(s)}\,P_{\alpha(s)}(-\beta) \tag{187}$$

For small ω

$$\beta_0 = \cos\omega \approx 1 - \omega^2/2 \tag{188}$$

$$P_{\alpha(s)}(-\beta_0) = P_{\alpha(s)}\left(-1+\frac{\omega^2}{2}\right) \tag{189}$$

Expanding (189) in a Taylor series about -1,

$$P_{\alpha(s)}\left(-1+\frac{\omega^2}{2}\right) = P_{\alpha(s)}(-1) + \frac{\omega^2}{2}\left(\frac{dP_{\alpha(s)}(\zeta)}{d\zeta}\right)_{\zeta=-1} + O(\omega^2/2) \tag{190}$$

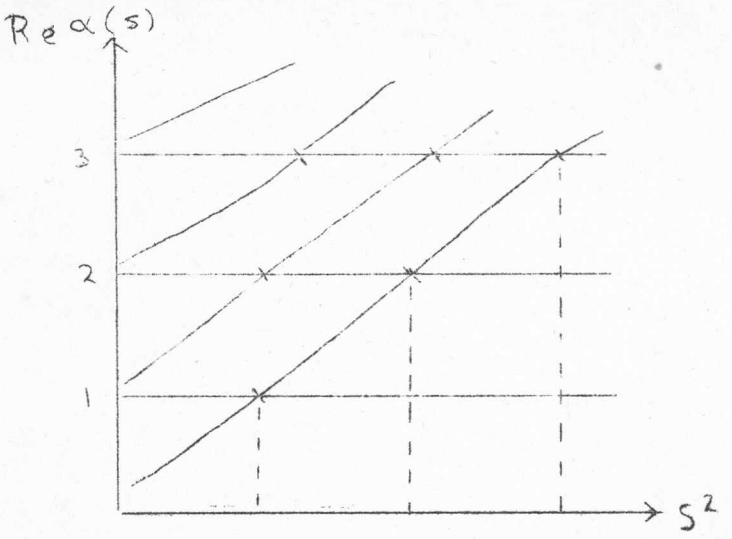
Now using equation (186) in conjunction with equations (187) and (190) and rearranging the resulting expression, we obtain

$$\omega^2 \approx -\frac{P_{\alpha(s)}(-1)}{\left[\frac{dP_{\alpha(s)}(\zeta)}{d\zeta}\right]_{\zeta=-1}} \tag{191}$$

Hence the motion of the pole at high energies controls the width of the diffraction peak.

Thus the observation of high energy scattering of elementary particles on each other, may reveal whether the interaction-dynamics is governed by a Regge type mechanism. The experimental results so far do not really substantiate these expectations. There are significant deviations from Regge behaviour for N-N scattering, and for π-N scattering the discrepancy is even worse. Nevertheless, it may be that there is some way of reconciling the experiments with Reggeology. Presumably we must be less naive in applying the basic ideas. For example, it is conceivable that in the relativistic case there are, apart from the moving Regge poles, also moving Regge branch cuts in the complex plane. At any rate, presently it is very difficult to make a final judgment.

On the other hand, Chew observed that elementary particles possess Regge type behaviour in the following sense. We can assume that elementary particles are resonances and bound states of some fundamental structure. Different Regge trajectories correspond then to different intrinsic quantum numbers.



The points of intersection of the straignt lines $Re\ \alpha(s) =$ integers give the energies at which elementary particles can occur. But only a few such points are confirmed experimentally.

Chapter VII.

CAUSALITY AND DISPERSION RELATIONS.

The preceding chapters have been based on the time-independent approach, which is quite satisfactory for the potential scattering problem. It will be recalled that the analyticity of the scattering amplitude depended on that of the Green's function. However one can also use a time-dependent approach for the study of analytic properties.

We make use of the causality principle in this new method. This principle becomes especially useful in quantum field theory, where in the Heisenberg picture, the operators and commutators are time-dependent. The causality principle enables us to deduce their analytic properties, which might otherwise have to be assumed.

Mathematical preliminaries:

Let $f(x)$ be a physical function of the real physical variable x. Let it have a fourier transform with respect to another variable t, given by

$$F(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-ixt}\, dx \qquad (192)$$

Let us further assume that $F(t)$ is a one-sided function, that is to say,

$$F(t) = 0 \text{ , if } t < 0 \qquad (193)$$

If t were the time variable, then $F(t)$ would be said to be a causal function.

From equation (193) we may deduce that the function $f(x)$ can be extended analytically to a complex argument $z = x + iy$ in

the upper half plane (Im z = y > 0) , and that f (z) is holomorphic in this region. To show this, we define the function f(z) as follows:

$$f(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(t)\, e^{izt}\, dt \qquad (194)$$

i.e.,

$$f(z) = \frac{1}{\sqrt{2\pi}} \int_{0}^{\infty} F(t)\, e^{ixt}\, e^{-yt}\, dt \qquad (195)$$

In the last step, zero was introduced as the lower limit by virtue of equation (193). The existence of equation (192) implies that the function F (t) must be bounded by a polynomial. The presence of the term e^{-yt} indicates that in the region y > 0 the integral always converges, that is to say, the function f (z) exists for Im z > 0 . Further, in a similar manner, we can establish the existence of the derivative f' (z) . Hence, we have defined an analytic regular function. For real values of z

$$f(x) = \lim_{y \to +0} f(z)$$

and this is valid at almost every point along the real axis.

This extension is by itself not sufficient to establish dispersion relations, since we know nothing about the asymptotic behaviour of f (z) . It may have a pole or an essential singularity at infinity. To avoid this, some restriction will have to be placed on the function f (x).

If f (x) is square integrable, i.e.,

$$\int_{-\infty}^{\infty} |f(x)|^2\, dx \qquad \text{exists,}$$

Titchmarsh has shown that the following four statements are equivalent*

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* E.C.Titchmarsh: ''Theory of Fourier Integrals''.

i) The Fourier transform obeys

$$F(t) = 0, \quad t < 0$$

ii) The function $f(x)$ is the limit of an analytic function when $y \to +0$ for almost all points on the real axis. The function $f(z)$ is regular in the upper half plane, and is such that

$$\int_{-\infty}^{\infty} |f(x+iy)|^2 dx < \text{constant, for every } y > 0 .$$

iii) The real part of $f(x)$ is a Hilbert transform of the imaginary part

$$\mathrm{Re}\ f(x) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\mathrm{Im}\ f(x')}{x' - x} dx'$$

iv) Similarly, the imaginary part is a Hilbert transform of $-\mathrm{Re}\ f(x)$

$$\mathrm{Im}\ f(x) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\mathrm{Re}\ f(x')}{x' - x} dx'$$

Any one of the above statements implies the others. That $f(x) = \lim_{y \to +0} f(z)$, follows from (i) while the latter part of (ii) is a consequence of Parseval's formula. Because of the square integrability of $f(z)$, the function itself must tend to zero for $|z| \to \infty$. Thus Cauchy's integral formula may be applied to yield the third and fourth statements.

By definition, a square integrable function whose Fourier transform vanishes for $t < 0$ is said to be a causal transform. The above discussion shows that causal transforms satisfy unsubtracted dispersion relations.

The restriction of square integrability is too strong when we seek to apply the above results to physical cases. A weaker restriction is then imposed — we require that $f(x)$ be bounded:

$$| f(x) | \leq \text{a constant.} \quad \text{(for real } x.)$$

Then as in Titchmarsh's theorem, we have four equivalent statements*.

(i) The Fourier transform obeys

$$F(t) = 0 , \quad t < 0$$

(ii) The function $f(x)$ is the limit of an analytic function $f(z)$ when $y \to 0$ for almost all points on the real axis. The function $f(z)$ is regular in the upper half plane and is bounded everywhere:

$$| f(z) | \leq \text{constant}, \quad \text{Im } z > 0 .$$

(iii) There is a subtracted dispersion relation

$$\text{Re } f(x) - \text{Re } f(x_0) = (x - x_0) \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{\text{Im } f(x')}{(x' - x)(x' - x_0)} dx'$$

where x_0 is any point on the real axis where $f(x)$ is regular.

(iv) Similarly

$$\text{Im } f(x) - \text{Im } f(x_0) = -(x - x_0) \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{\text{Re } f(x')}{(x' - x)(x' - x_0)} dx'$$

where x_0 is the same as the point described above.

Again any one of the statements implies the others.

We make a few comments concerning the proofs. Since it has only been assumed that $f(x)$ is a bounded function, we know nothing about the asymptotic behaviour of $f(z)$ for $| z | \to \infty$. However, if we define a new function:

$$\Phi(z) = \frac{f(z) - f(x_0)}{z - x_0}$$

then it can be shown that $\Phi(z) \to 0$ when $| z | \to \infty$. The

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* J.S. Toll , Phys. Rev. 104, 1760 (1956).

function $f(z)$ is regular in the upper half plane, as a consequence of the first statement of Toll's theorem, and therefore, $\Phi(z)$ is also regular. Cauchy's integral formula may now be applied to the function $\Phi(z)$, and hence the subtracted dispersion relations are obtained.

If a function $f(x)$ is bounded and if its Fourier transform vanishes for $t < 0$, then $f(x)$ is said to be a causal factor. The Toll theorem shows that causal factors satisfy once subtracted dispersion relations.

The reason why $f(x)$ is called a causal factor is as follows. Let $g_1(x)$ be any causal transform, that is, let it be square integrable along the real axis and let its Fourier transform vanish for $t < 0$. Let $f(x)$ be a causal factor in the sense explained above. Then the product:

$$g_2(x) = f(x)\ g_1(x)$$

is also a causal transform. This may be surprising, since, in general, if two factors exist, one with a strong property and the other with a weak property, then the product has the weaker property. However, in this particular case, the product must be square integrable along the real axis due to the presence of $g_1(x)$. Moreover, since $f(x)$ and $g_1(x)$ may both be extended to the complex plane for $\mathrm{Im}\ z > 0$ and since $g_1(z) \to 0$ for large values of $|z|$, we have $g_2(z) \to 0$ as $|z| \to \infty$. Therefore Cauchy's integral formula may be used to find $g_2(z)$ at any point in $\mathrm{Im}\ z > 0$ and this leads to the unsubtracted dispersion relation

$$\mathrm{Re}\left[f(x)\, g_1(x)\right] = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\mathrm{Im}\, f(x')\, g_1(x')}{x' - x}\, dx'$$

But by Titchmarsh's theorem, this is equivalent to stating that the Fourier transform of $g_2(x)$ is one-sided. Therefore $g_2(x)$ is a causal transform. The role of $f(x)$ is then essentially that of a factor relating two causal transforms.

The converse is also true. That is, if we have a function $f(x)$ whose Fourier transform $F(t)$ vanishes for $t < 0$ and which is given by

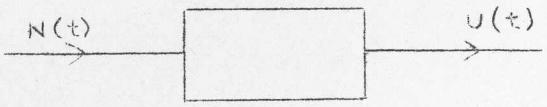
$$f(x) = \frac{g_2(x)}{g_1(x)}$$

where $g_1(x)$ and $g_2(x)$ are causal transforms, then $f(x)$ is a causal factor, that is, it is bounded for all x.

It has been shown, by Toll that the conditions on $f(x)$ may be relaxed further, and that one can still obtain dispersion relations with, however, more subtractions. This is useful even in quantum field theory when highly singular functions are met with, such as the δ-function or its derivatives. They pose no serious problem to establishing dispersion relations.

Application to Physical Systems:

We start with a most general physical system wherein the causality principle is applied. Let us consider a ''black box'', that is, a system about whose intrinsic properties we know nothing. An input $N(t)$ is fed into the system



and an output $U(t)$ is observed. Here t is the time variable.

This information is obviously useless as it stands. We must, therefore, impose some general restrictions which define the physical behaviour of the system:

(i) The system must be linear, that is, the output must be a linear function of the input. (A typical example is the electrical network in which an input voltage and output current are linear functions of each other.) Mathematically this type of restriction implies that $U(t)$ and $N(t)$ are connected by a linear differential or integral equation. The general solution to this equation can be written

$$U(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(t,t')\, N(t')\, dt' \qquad (196)$$

where $F(t, t')$ is the Green's function for the differential operator. Effectively, $U(t)$ is a linear transform of $N(t)$.

(ii) The system must be steady. This means that the characteristics of the system itself do not vary in time, even though the input may do so. Therefore if the origin of the time scale is changed, the equations governing the system must remain unaffected. Consequently, the function $F(t, t')$ must be of the form $F(t-t')$ and consequently equation (196) should be written as

$$U(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(t-t')\, N(t')\, dt' \qquad (197)$$

In the case of the electrical network, F is the complex impedence when the network is passive.

(iii) The system must be causal. To put this more explicitly, we demand that no output can occur <u>before</u> the input was applied. If the input starts only at the instant $t = 0$, then no output exists for $t < 0$. From equation (197), we must have

$$F(t) = 0, \quad t < 0 \qquad (198)$$

It may be thought that this equation is merely equivalent to a statement about the unidirectional flow of time. This is an erroneous idea. One cannot assume that equation (198) necessitates the retarded Green's function only, because if the system is invariant under time reversal (changing + t to - t), then both the retarded and the advanced Green's functions are physically meaningful. However, in a physical situation, we usually wish to determine the present state of the system from a knowledge of its past states. In such a case we must use only the retarded Green's function. If a situation arises where we require the past state from a knowledge of the present, then the advanced solution has to be used, that is, $F(t) = 0$ for $t > 0$ *.

The Fourier transform of the Green's function may be written as:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(t)\, e^{ixt}\, dt \qquad (199)$$

From the causal nature of $F(t)$ it then follows that the function $f(x)$ may be analytically extended to the upper half of the complex domain of z ($z = x + iy$). In quantum field theory, singularities may occur but still one can analytically extend $f(x)$.

The causality principle thus shows that the Fourier transform of the Green's function is analytic in the upper half plane. However, this gives no information about its asymptotic behaviour as $z \to \infty$. Therefore we cannot write a dispersion relation unless some further restriction is imposed on the system. This leads us to the final assumption, viz.,

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* For details, see J.Hilgevoord: 'Dispersion Relations and Causal Description'',Chap.I.

(iv) The system must be such that an arbitrary square integrable input produces a square integrable output. This is quite a strong condition. It requires that

$$\text{if} \quad \int_{-\infty}^{\infty} |N(t)|^2 \, dt \quad \text{exists} \qquad \text{then} \quad \int_{-\infty}^{\infty} |U(t)|^2 \, dt \quad \text{also exists.} \tag{200}$$

In many cases, even if the differential equation cannot be solved, or if the explicit form of the Green's function cannot be found, still the above can be verified. For instance, in an optical problem or in a transmission system, the integrable merely correspond to the total input and output energies. In scattering theory, N (t) and U (t) are wave functions and hence square integrable.

This final assumption can be used to show that f (x) is a causal factor. Let us define the Fourier transform of N (t) and U (t) :

$$n(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} N(t) \, e^{ixt} \, dt \tag{201}$$

$$u(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} U(t) \, e^{ixt} \, dt \tag{202}$$

Because of (200), these transforms exist, and they are also square integrable functions.

Now the convolution of two functions g and h is defined as

$$g \cdot h = \int_{-\infty}^{a} g(\xi) \, h(\alpha - \xi) \, d\xi \tag{203}$$

where the integration is carried out over the whole of the range of α ($-a < \alpha < +a$). By the convolution theorem, the Fourier transform of g . h is simply the product of the individual Fourier transforms of g and h .

Equations (197) and (203) are ''similar''. Using (199), (201) and (202) and the convolution theorem, we can directly write

$$u(x) = f(x)\ n(x) \qquad (204)$$

For the sake of clarity let us assume that the input is switched on at the moment $t = 0$, that is, $N(t) = 0$ for $t < 0$. This together with (200) implies that $n(x)$ is a causal transform. Moreover, from (197) we see that $U(t) = 0$ also, for $t < 0$. Therefore $u(x)$ is also a causal transform. Then equation (204) shows that $f(x)$ is a ratio of two causal transforms. We already know that $f(x)$ is such that its Fourier transform $F(t) = 0$ for $t < 0$. Then, by virtue of the ''converse theorem'' stated towards the end of the preceding section, $f(x)$ must be a causal factor. In other words, $f(x)$ must be bounded, and Toll's theorem immediately leads to a dispersion relation for $f(z)$.

(Note: The above assumption, about $N(t)$ being a causal function, is no restriction on the system. The system itself is independent of the input or output, and therefore $f(x)$ will always be a causal factor. The actual restriction arises from a different cause. Since $f(x) = u(x) / n(x)$ the function $f(x)$ exists only if $n(x) \neq 0$ everywhere. Therefore the arbitrary free input must be such that in addition to being square integrable, its Fourier transform must never vanish. There is, however, a wide class of functions which satisfy this, so that the restriction is not at all a serious one.)

It may be seen that there exists a definite connection between causality and dispersion relations by means of the following argument. Let $N(t) = 0$ for $t < 0$. This condition may be

interpreted as being due to the existence of a relationship between the amplitude and phase parts of the complex Fourier coefficients $n(x)$, such that prior to $t = 0$, they cancel each other and effectively produce a zero input signal. But from equation (197) we also have $u(t) = 0$ for $t < 0$, which means that the Fourier coefficients $u(x)$ also satisfy some such relationship between the amplitude and phase parts. Therefore from equation (204),

$$u(x) = f(x)\ n(x),$$

we see that the amplitudes and phases of $f(x)$ are not arbitrary but must also satisfy some relationship between themselves. But an equation between an amplitude term and a phase term is equivalent to an equation between real and imaginary parts, and this is just what a dispersion relation amounts to.

To summarise this section, what we have done is to impose four conditions on a physical system. From these conditions, we have shown that the Fourier transform of the Green's function which links up the input and output, is bounded on the real axis, and that it can be analytically extended to the upper half plane.

Application to Potential Scattering:

In Chapter III, we solved the time independent Schrodinger equation for potential scattering by introducing a Green's function $g_J(\underline{r}, \underline{r}'; k)$. The analytic properties of this function determined those of the scattering amplitude $f(s, t)$, and these properties were studied by using the spectral representation of $g_J(\underline{r}, \underline{r}'; k)$ (Ref. equation 53). It can now be shown that the principle of causality also can be a starting point for studying the properties of g_J.

The dynamical equation for non-relativistic potential scattering is

$$\left[\frac{\hbar}{i}\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\nabla^2 + V(\underline{r},t)\right]\psi(\underline{r},t) = 0 \qquad (205)$$

Here $\psi(\underline{r},t)$ is the complete solution of the wave equation, and $V(\underline{r},t)$ is an arbitrary potential. In practice, we take V to be a switched potential, which is non-zero and constant (in time) only for a finite interval of time, and zero otherwise, that is,

$$V(\underline{r}\ t) = \begin{cases} V_0(\underline{r}), & 0 < t < \tau \\ 0, & t < 0 \text{ and } t > \tau \end{cases} \qquad (206)$$

We should now express the output as an integral transform of the incident wave, so as to obtain a relation of the type (196). To do so, we first separate the solution ψ into the incident wave $\varphi(\underline{r},t)$ and the scattered wave $\Phi(\underline{r},t)$:

$$\psi(\underline{r},t) = \varphi(\underline{r},t) + \Phi(\underline{r},t) \qquad (207)$$

The incident wave must satisfy the dynamical equation in the case when there is no potential

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\nabla^2\right)\varphi(\underline{r},t) = 0 \qquad (208)$$

We choose as a particular solution, a plane wave travelling in a direction specified by the momentum vector $\underline{k}_0$:

$$\varphi(\underline{r},t) = e^{i\underline{k}_0\cdot\underline{r}}\, e^{-\frac{i}{\hbar}E_0 t} \qquad (209)$$

where $E_0 = \frac{\hbar^2 k_0^2}{2m}$. Substituting (207) in equation (205),

and taking note of (208), we have

$$\left(\frac{\hbar}{i} \frac{\partial}{\partial t} - \frac{\hbar^2}{2m} \nabla^2 + V \right) \Phi = - V \varphi \qquad (210)$$

This is a standard linear differential equation, with a known source term on the right hand side and the unknown function Φ on the left. The equation is solved by using the appropriate Green's function which satisfies

$$\left(\frac{\hbar}{i} \frac{\partial}{\partial t} - \frac{\hbar^2}{2m} \nabla^2 + V \right) \mathcal{K}(\underline{r}, t) = -\delta(r)\, \delta(t) \qquad (211)$$

Hence the solution to (210) is

$$\Phi(\underline{r}, t) = \int \int_{-\infty}^{\infty} \mathcal{K}(\underline{r}, \underline{r}'; t, t')\, V(\underline{r}', t')\, \varphi(\underline{r}', t')\, dt'\, d^3\underline{r}'$$

From the constancy of the coefficients and from the hermiticity of the differential operators, it follows that $\mathcal{K}$ depends only on $(\underline{r} - \underline{r}')$ and $(t - t')$. Hence the above equation must be written

$$\Phi(\underline{r}, t) = \int \int \mathcal{K}(\underline{r} - \underline{r}', t - t')\, V(\underline{r}', t')\, \varphi(\underline{r}' t')\, dt'\, d^3\underline{r}' \qquad (212)$$

This solution is not definite, unless $\mathcal{K}$ satisfies a boundary condition at least in t, such that Φ also obeys the necessary boundary condition. Here the causality principle is introduced.

The actual formulation is as follows. The scattered wave function $\Phi(\underline{r}, t)$ on the surface of any sphere described around the scattering centre at any instant t, must depend only on those values of $\varphi(\underline{r}, t)$ on this sphere occurring before the instant t. This is physically obvious, since the scattered wave must appear only after the incident wave. However, the condition is not very strong, and therefore its application does not carry us very far.

In any case, the condition requires, by virtue of equation (212), that

$$\mathcal{K}(\underline{r},t) = 0 \quad , \quad t < 0 \tag{213}$$

It is this relation that forms the basis of our present discussion.

We denote the solution (213) by $\mathcal{K}^+$ to indicate that it is the retarded Green's function. To evaluate this, we use the unperturbed Green's function $K(\underline{r},t)$ which satisfies the equation

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\nabla^2\right) K(\underline{r},t) = -\delta(\underline{r})\,\delta(t) \tag{214}$$

Equation (212) is rewritten as

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\nabla^2\right)\mathcal{K}(\underline{r},t) = -\delta(\underline{r})\,\delta(t) - V(\underline{r},t)\,\mathcal{K}(\underline{r},t) \tag{215}$$

From the preceding equations, we have an integral equation for $\mathcal{K}$:

$$\mathcal{K}(\underline{r},t) = K(\underline{r},t) + \int_{-\infty}^{\infty}\int K(\underline{r}-\underline{r}',t-t')\,V(\underline{r}',t')\,\mathcal{K}(\underline{r}',t')\,dt'\,d^3\underline{r}' \tag{216}$$

If the function K is known; then $\mathcal{K}$ may be found from the above equation. It is a Fredholm type of integral equation whose solution can be written using the Neumann series method:

$$\begin{aligned}\mathcal{K}(\underline{r},t) = K(\underline{r},t) &+ \iint K(\underline{r}-\underline{r}',t-t')\,V(\underline{r}',t')\,K(\underline{r}',t')\,dt'\,d^3\underline{r}' \\ &+ \iiiint K(\underline{r}-\underline{r}',t-t')\,V(\underline{r}',t')\,K(\underline{r}'-\underline{r}'',t'-t'') \\ &\qquad V(\underline{r}'',t'')\,K(\underline{r}'',t'')\,dt''\,dt' \\ &\qquad d^3\underline{r}''\,d^3\underline{r}' \\ &+ \cdots\end{aligned} \tag{217}$$

This is effectively the Born approximation series.

We now make use of the fact that V is a switched potential. We see that if $\mathcal{K}$ must satisfy (213), then K must be the retarded Green's function K^+, that is, the unperturbed Green's function must be such that

$$K^+ (\underline{r} , t) = 0 , t < 0 \qquad (218)$$

The function K^+ must be determined explicitly. Once this is done, the solution ψ^+ may be written down:

$$\psi^+(\underline{r},t) = \varphi(\underline{r},t) + \iint \mathcal{K}^+(\underline{r}-\underline{r}',t-t')\, V(r't')\, \varphi(\underline{r}'t')\, dt'\, d^3\underline{r}' \qquad (219)$$

The n'th approximation for $\mathcal{K}^+$ then gives the n'th approximation of $\psi^+(\underline{r},t)$

To determine K^+, we start with a general theorem. Suppose we have an arbitrary differential operator of the form:

$$\Omega = a_0 + a_1 \frac{\partial}{\partial x_1} + \cdots + a_n \frac{\partial}{\partial x_n} + a_{11} \frac{\partial^2}{\partial x_1^2} + a_{12} \frac{\partial^2}{\partial x_1 \partial x_2} + \cdots + a_{nn} \frac{\partial^2}{\partial x_n^2} + \cdots + a_{\underbrace{nn\ldots n}_{(r)}} \frac{\partial^r}{\partial x_n^r} \qquad (220)$$

The operator Ω contains an arbitrary number of differential coefficients. Let the coefficients a_0, a_1, etc. be constants. If the Green's function corresponding to Ω is $F (x_1 \ldots\ldots x_n)$:

$$\Omega F(x_1 \cdots x_n) = -\delta(x_1) \cdots \delta(x_n) \qquad (221)$$

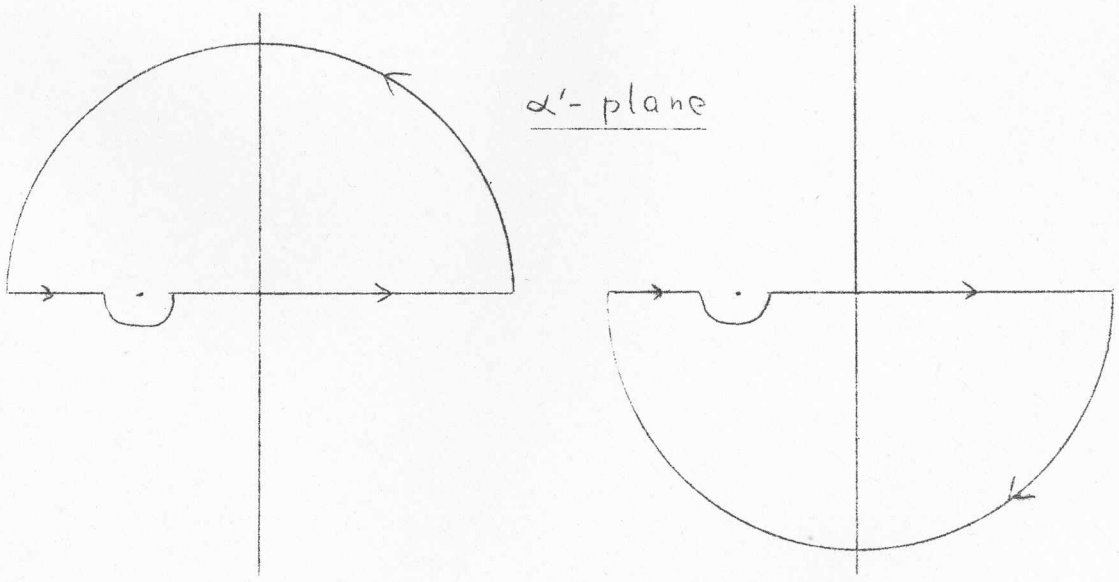
then F is given by

$$F(x_1 \cdots x_n) = -\frac{1}{(2\pi)^n} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \frac{e^{i(k_1 x_1 + \cdots + k_n x_n)}\, dk_1 \cdots dk_n}{a_0 + a_1(ik_1) + \cdots a_n(ik_n) + a_{11}(ik_1)^2 + \cdots + a_{nn\cdots n}(ik_n)^r} \tag{222}$$

Here the integration is performed along the real axis for each variable. If poles occur on the real axis, then the contour must be defined in such a way as to fit the solution to the given boundary conditions. Equation (214) can be solved by this method, so as to yield

$$K(\underline{r}, t) = -\frac{1}{(2\pi)^4 \hbar} \int\int_{-\infty}^{\infty} \frac{e^{i\underline{k}'\cdot\underline{r}}\, e^{i\alpha' t}}{\alpha' + \frac{\hbar}{2m} k'^2}\, d\alpha' d^3\underline{k}' \tag{223}$$

We first integrate with respect to α'. It is then seen that the integrand has a pole at $\alpha' = -\frac{\hbar}{2m} k'^2$. This pole must be circumvented in such a way that the solution is the retarded Green's function, K^+.



(i) $t > 0$ (ii) $t < 0$

It will be proved a little later that the correct modification is to circumvent the pole from below. The contour is closed in the upper half plane if t is positive, and in the lower half plane if t is negative. In both cases it is such that the integrand vanishes at infinity and that the contribution from the large semi-circle is zero. However, in the former case the pole is included inside the contour, and using the residue theorem, the integration over α' will yield

$$2\pi i \; e^{-i\hbar k'^2 t/2m} \quad , \; t > 0$$

In the latter case, the pole is excluded, and so the integral is zero. Therefore (223) takes the form

$$K^+(\underline{r}, t) = -\frac{1}{(2\pi)^3} \frac{i}{\hbar} \Theta(t) \int e^{i \underline{k}' \cdot \underline{r}} \, e^{-i \frac{\hbar k'^2}{2m} t} \, d^3\underline{k}' \qquad (224)$$

where

$$\Theta(t) = \begin{cases} 1 \; , & t > 0 \\ 0 \; , & t < 0 \end{cases}$$

We are justified in our choice of the contour, since the solution vanishes for $t < 0$, and it is therefore written K^+.

The integration over k' space is straightforward, and the final expression is

$$K^+(\underline{r}, t) = \frac{\Theta(t)}{i\hbar} \left(\frac{m}{2\pi i \hbar t} \right)^{3/2} \exp\left(\frac{im}{2\hbar} \frac{|\underline{r}|^2}{t} \right) \qquad (225)$$

Now, rewriting (210) as

$$\left(\frac{\hbar}{i} \frac{\partial}{\partial t} - \frac{\hbar^2}{2m} \nabla^2 \right) \Phi = -V \Psi$$

and using (214), we can directly write

$$\Phi(\underline{r},t) = \int\int_{-\infty}^{\infty} K(\underline{r}-\underline{r}',t-t')\, V(\underline{r}',t')\, \psi(\underline{r}',t')\, dt'\, d^3\underline{r}'$$

substituting (225) into the above equation, we finally have

$$\psi(\underline{r},t) = e^{i\underline{k}_0\cdot\underline{r}}\, e^{-\frac{i}{\hbar}E_0 t} + \frac{1}{i\hbar}\int\int_{-\infty}^{\infty} \theta(t-t')\left[\frac{m}{2\pi i\hbar(t-t')}\right]^{3/2} \exp\left[\frac{im}{2\hbar}\frac{|\underline{r}-\underline{r}'|^2}{t-t'}\right] V(\underline{r}',t')\,\psi(\underline{r}',t')\, dt'\, d^3\underline{r}' \qquad (226)$$

The θ function reflects the causality property. The value of $\psi(\underline{r},t)$ for any instant t depends only on those values of $\psi(\underline{r}',t')$ for which $t > t'$.

Equation (226) represents the outgoing wave, as required. This can be seen by taking the limit as $r \to \infty$ and $t \to \infty$, when a factor $\exp\left(\frac{im}{2\hbar}\frac{r^2}{t}\right)$ can be extracted from the integral. This obviously represents an outgoing spherical wave, since r must increase with the time t. We may therefore write the solution to (226) as $\psi^+(\underline{r},t)$.

Though equation (226) is nothing but an integral equation corresponding to the differential equation (205), the former is easier to deal with and approximations made with this equation may be better than those made in the case of the differential equation.

It can now be shown that the time-independent Green's function G and the time-dependent Green's function $\mathcal{K}$ are connected by a Fourier transformation.

Let us first take the function K as defined in the equation (223). Let both sides be multiplied by $e^{iEt/\hbar}$ and integrated over t. Using the relation

$$\int_{-\infty}^{\infty} \exp\left[i\left(\alpha' + \frac{E}{\hbar}\right)t\right] dt = 2\pi\,\delta\left(\alpha' + \frac{E}{\hbar}\right) \qquad (227)$$

and performing the integration over α', we have

$$\int_{-\infty}^{\infty} K(\underline{r},t)\, e^{\frac{i}{\hbar}Et}\, dt = -\frac{1}{(2\pi)^3 \hbar} \int \frac{e^{i\underline{k}'\cdot\underline{r}}}{\frac{\hbar}{2m}k'^2 - \frac{E}{\hbar}}\, d^3\underline{k}' \qquad (228)$$

So far E has been treated as a parameter. It is now identified with the energy of the scattering system. If no bound states occur, then

$$E = \frac{\hbar^2 k^2}{2m} \qquad (229)$$

Substituting this in equation (228), we have

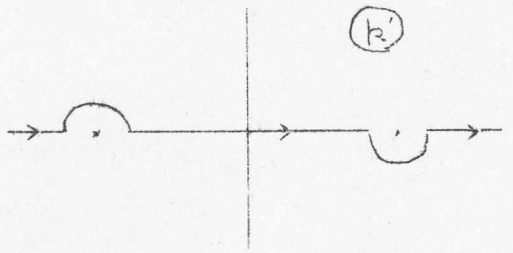
$$\int_{-\infty}^{\infty} K\, e^{\frac{iEt}{\hbar}}\, dt = -\frac{2m}{\hbar^2}\,\frac{1}{(2\pi)^3} \int \frac{e^{i\underline{k}'\cdot\underline{r}}}{k'^2 - k^2}\, d^3\underline{k}' \qquad (230)$$

The right hand side of this equation is, but for the factor $\left(-\frac{2m}{\hbar^2}\right)$ the Green's function for the unperturbed differential equation

$$\left(\nabla^2 + k^2\right) G(\underline{r};k) = -\delta(\underline{r})$$

Therefore (230) can be written as

$$\int_{-\infty}^{\infty} K(\underline{r},t)\, e^{iEt/\hbar}\, dt = -\frac{2m}{\hbar^2}\, G(\underline{r};k) \qquad (231)$$



Now, in the evaluation of G, two poles at $k' = \pm k$ are encountered. If we desire to compute the outgoing Green's function G^+, then the poles must be circumvented as shown in the figure. This procedure is equivalent to circumventing the pole of equation (223) from below, which lead to the retarded Green's function K^+. Therefore

$$\int_{-\infty}^{\infty} K^+(\underline{r},t)\, e^{iEt/\hbar}\, dt = -\frac{2m}{\hbar^2}\, G^+(\underline{r},k) \qquad (232)$$

that is, the outgoing stationary Green's function G^+ is the Fourier transform of the retarded time-dependent Green's function K^+.

Next, let us multiply both sides of the equation (216) by $e^{iEt/\hbar}$ and integrate over t. On the left we obtain the Fourier transform of K denoted by $\mathcal{F}[K(\underline{r},t)]$. Using the relation

$$\int_{-\infty}^{\infty} K(\underline{r}-\underline{r}',t-t')\exp\left(\frac{i}{\hbar}Et\right)dt = -\frac{2m}{\hbar^2}\, G(\underline{r}-\underline{r}';k)\exp\left(\frac{i}{\hbar}Et'\right)$$

and integrating over t' on the right hand side, we have with the aid of (231),

$$\mathcal{F}[K(\underline{r},t)] = -\frac{2m}{\hbar^2}\, G(\underline{r},k) - \frac{2m}{\hbar^2}\int G(\underline{r}-\underline{r}';k)\, V(\underline{r}')\, \mathcal{F}[K(\underline{r}',t')]\, d^3\underline{r}' \qquad (233)$$

We have here replaced $V(\underline{r}', t')$ by $V(\underline{r}')$ since this is the value of the potential over the effective interval $0 < t' < \tau$ of the integration over t'.

Equation (233) may be compared with equation (44):

$$-g(\underline{r},\underline{r}';k) = G(\underline{r},\underline{r}';k) + \int G(\underline{r},\underline{r}''k)V(\underline{r}'')g(\underline{r}''\underline{r}'k)\,d^3\underline{r}''$$

The two integral equations are identical, so that we can write

$$\int_{-\infty}^{\infty} K(\underline{r},t)\exp\left(\frac{i}{\hbar}Et\right)dt = \frac{2m}{\hbar^2}\,g(\underline{r},k) \qquad (234)$$

Corresponding to (232), we also have

$$\int_{-\infty}^{\infty} K^+(\underline{r},t)\exp\left(\frac{i}{\hbar}Et\right)dt = \frac{2m}{\hbar^2}\,g^+(\underline{r},k) \qquad (235)$$

This equation may be inverted to obtain

$$K^+(\underline{r},t) = \frac{m}{\pi\hbar^2}\int_0^{\infty} g^+(\underline{r},k)\exp\left(-\frac{i}{\hbar}Et\right)dE \qquad (236)$$

This is true only if no bound states occur, since this has already been assumed, together with $E = \hbar^2k^2/2m$. If bound states do occur, then all the possible bound states with energies E_b must also be taken into account. This is done by rewriting equation (236) as

$$K^+(\underline{r},t) = \frac{m}{\pi\hbar^2}\int_0^{\infty} g^+(\underline{r},k)\exp\left(-\frac{i}{\hbar}Et\right)dE + \frac{m}{\pi\hbar^2}\sum_{b=1}^{N} g^+\left(\underline{r},\sqrt{|E_b|}\right)\exp\left(-\frac{i}{\hbar}E_bt\right) \qquad (237)$$

The physical interpretation of (237) is as follows. Since K^+ is a solution of the dynamical equation for scattering, it can be expanded in terms of the energy eigenfunctions. Equation (236) then merely expresses K^+ in the energy representation, and is equivalent to an eigenfunction of the continuous spectrum. When there are bound states, the integral must be supplemented by a sum over these states, so as to lead to equation (237).

If equation (237) is now inverted, it will be seen that $\mathcal{G}_j^+$ is no longer the Fourier transform of a causal function $\mathcal{K}^+$. Instead there is an additional term

$$\int_{-\infty}^{\infty} \left(\sum_b \mathcal{G}^+(\underline{r}, \sqrt{|E_b|}) e^{-\frac{i}{\hbar} E t} \right) dt$$

which does not vanish when $t < 0$. We must therefore study afresh the analytic properties of $\mathcal{G}^+$.

When no bound states occur, we note that $\mathcal{G}^+$ is the Fourier transform of the function $\mathcal{K}^+$ which is zero for $t < 0$, on account of the causality principle. Therefore $\mathcal{G}^+$ can be analytically extended into the upper half of the complex energy plane. Moreover, it is a causal factor. This can be seen by comparing equation (212) with equation (197). Now $V\varphi$ can be considered as an input and Φ as an output. Both the square integrable with respect to time, for

$$\int_{-\infty}^{\infty} |\varphi(\underline{r}, t)|^2 \, dt$$

and

$$\int_{-\infty}^{\infty} |\Phi(\underline{r}, t)|^2 \, dt$$

are respectively the mean times for the incident and scattered particle spent at the point $\underline{r}$ and therefore finite. Hence $\mathcal{G}^+$ the Fourier transform of $\mathcal{K}^+$ is a ratio of two causal transforms, and consequently is a causal factor by itself. Therefore a once-subtracted dispersion relation for $\mathcal{G}^+$ exists, and hence for the scattering amplitude $f(s, t)$.

When bound states exist, equation (237) shows that there is a sum of terms which does not vanish for $t < 0$. This is simply interpreted as giving rise to the pole terms in the dispersion relation.

Finally, we observe that we have proved the existence of a connection between causality and dispersion relations. The former implies the latter. However, we also note that causality was not absolutely necessary to study the analytic properties of g^+. In fact, the approach in this chapter is not very useful because the precise form of the dispersion relations is obtained only if explicit properties of the potential $V(r)$ are also taken into account. The reason is that the causality condition itself is not strong enough.

The situation is better in relativistic theory. Here the velocity of any particle cannot exceed that of light, and this gives a stronger condition. For example in the case of the Kramers-Kronig relation, we use the electromagnetic scattering Green's function $E(r, t)$ which must ganish for all $t < r/c$. Then $n(\omega) - 1$ can be directly shown to be a causal factor, and the subtracted dispersion relation willffollow.

The causality condition finds greatest application to dispersion relations in quantum field theory and the relativistic theory of elementary particles, where, in fact, it was for a long time, the only suitable method of approach. It is also useful in the non-relativistic many-body problem.

Chapter VIII.

THE S-MATRIX.

Our previous treatment has been restricted explicitly to potential scattering. We now attempt to generalise the theory so as to encompass all possible physical processes involving collisions. This necessitates the introduction of the S-matrix.

The concept of the S-matrix took shape after Heisenberg, in 1943, enquired into the possible experimental facts which could be related directly to a collision theory. These are basically three: i) the character of the particles long ''before'' and long ''after'' collision, ii) the bound states of the system, iii) the cross sections for ordinary elastic scattering as well as for processes where the internal character of the particles is changed. (The process is then generally referred to as a reaction.)

The character of the system before or after the collision may be described by state vectors, and the interaction itself may be embodied in a ''black box'' which transforms an input state into an output state. Thus the particular nature of the process is relegated to the back-ground, and the system is characterised by the transforming operators known as the scattering operator or S-operator. If represented in terms of a set of base-vectors, it is called the S-matrix.

The effect of the S-operator is defined by

$$\Psi^{out} = S\,\Psi^{in} \tag{238}$$

where Ψ^{in} and Ψ^{out} are the ''input'' and ''output'' states.

The explicit form of S will depend on the mode of approach -- whether time-independent or time-dependent. For the time-dependant approach, one may again employ either the Heisenberg or the interaction pictures, consequently these will result in three explicit definitions of the S-operator.

We shall adopt the time-independent approach. For convenience, we shall take a set of orthonormal states:

$$| a \rangle , | b \rangle , \ldots | i \rangle, \ldots | f \rangle, \ldots | n \rangle , \ldots$$

which form a complete set, of eigenstates in a Hilbert space, corresponding to a maximal set of simultaneous observables, and to which will generally depend on the parameters of the problem.

By taking the projections on some state $| n \rangle$ of Ψ^{in} and Ψ^{out} we define

$$\langle n | \Psi^{in} \rangle \equiv \Psi^{+} \tag{239a}$$

$$\langle n | \Psi^{out} \rangle \equiv \Psi^{-} \tag{239b}$$

Our aim must be to determine the Ψ^{+} and Ψ^{-} and from them the S-operator, from which we can deduce the cross-sections.

Let us first study the S-matrix and its general properties. First, the S-matrix must be a unitary operator. This follows from the requirement that if the input is normalisable, so also is the output, since the norms must be equal because of the conservation of probability:

$$| \Psi^{in} |^2 = | \Psi^{out} |^2 = 1$$

It follows from (238) that

$$(\Psi^{out}, \Psi^{out}) = (\Psi^{in}, S^{*} S \Psi^{in})$$

Therefore

$$S^* S = 1 . \tag{240a}$$

Also $$\left(S^{-1} \Psi^{out}, S^{-1} \Psi^{out} \right) = \left(\Psi^{in}, \Psi^{in} \right)$$

from which

$$S S^* = 1 \tag{240b}$$

Equations (240) then define the unitarity of the S-matrix.

Another property of the S-matrix is that it must satisfy the causality principle. With this is connected its analytic behaviour.

The S-matrix must also satisfy the symmetry properties of the system, such as gauge invariance or, in a relativistic system, Lorentz invariance.

These properties of the S-matrix are probably too general to be of <u>direct</u> use. Therefore we employ a more modest approach and start with the assumption that the Hamiltonian and the Schrödinger equation exist, and that the operator S can be derived from them. We now obtain expressions for the transition probabilities in terms of S.

Let us suppose that the input state is one of the eigenkets $|\, i \,\rangle$. The out-going state can then be a linear superposition of all such states.

$$\Psi^{out} = \sum_n C_n |\, n \rangle \tag{241}$$

where C_n represents the transition amplitude to some state specified by $n \neq i$. Suppose we require the probability for a

transition to $| f >$. Then

$$C_f = \langle f | \Psi^{out} \rangle$$
$$= \langle f | S \Psi^{in} \rangle$$
$$= \langle f | S | i \rangle$$
$$= S_{fi} \qquad (242)$$

which is the matrix element with respect to the same base as that in which the input and output are expressed. This however will not directly give the transition probability, to obtain which, certain manipulations have yet to be performed.

The physically interesting transitions are those for which the initial and final states are different and therefore we exclude the $i \to i$ transitions by subtracting the unit matrix from S. In this new matrix, we can again take out a factor $\delta (E_i - E_f)$, since we are interested only in reactions for which energy is conserved. Then we write:

$$S_{fi} = \delta_{fi} - 2\pi i \, \delta(E_i - E_f) T_{fi} \qquad (243)$$

The constant $(- 2 \pi i)$ is chosen for convenience. Equation (243), then defines the elements of a new matrix T. In equation (243), one must not be confused over the meaning of the two δ-functions. The first, δ_{fi} vanishes for $i \neq f$, where i and f denote <u>all</u> the quantum numbers associated with the system. The Dirac delta-function $\delta (E_i - E_f)$ only indicates that while transitions between different states take place, the energies in the two states must be the same. We now consider only those transitions

for which $i \neq f$. For convenience, we choose a new function defined by

$$S_{fi}^{\tau} = -T_{fi}\,\frac{i}{\hbar}\int_{-\frac{\tau}{2}}^{+\frac{\tau}{2}} e^{\frac{i}{\hbar}(E_i - E_f)t}\,dt \qquad (244)$$

Then

$$S_{fi} = \lim_{\tau \to \infty} S_{fi}^{\tau} \quad \text{for } f \neq i \qquad (245)$$

The transition probability per unit time can then be written as

$$\omega_{i \to f} = \lim_{\tau \to \infty} \frac{|S_{fi}|^2}{\tau} \qquad (246)$$

substituting for S_{fi}^{τ} and using the relation

$$\delta(\alpha) = \frac{1}{\pi} \lim_{x \to \infty} \frac{\sin^2 \alpha x}{\alpha^2 x}$$

we can write

$$\omega_{i \to f} = \frac{2\pi}{\hbar}\,\delta(E_i - E_f)\,|T_{fi}|^2 \qquad (247)$$

We may note that this form was easily derived by using the expression (244). Had we directly used S_{fi} we would have to deal with terms like $[\delta(E_i - E_f)]^2$, which have been eliminated in this procedure.

We actually require the transition not into a sharp state $|f\rangle$, but into a group of states around $|f\rangle$ having nearly equal energies. Denoting as usual, the density of states around E_f by the symbol $\rho(E_f)$, the transition probability is

$$\omega = \frac{2\pi}{\hbar}\int_{E_f - \Delta E/2}^{E_f + \Delta E/2} \delta(E_i - E_f)\,|T_{fi}|^2\,\rho(E_f)\,dE_f$$

$$= \frac{2\pi}{\hbar}\,\rho(E_f)\,|T_{fi}|^2 \qquad (248)$$

This has the same structure as Fermi's golden rule, but has the advantage of being an exact formula, whereas the 'golden rule' is an approximate one. However, for computational purposes, approximations have to be introduced usually.

Finally we can define the reaction matrix T, on the energy shell,

$$\left(\underline{T}\right)_{fi} = -2\pi i\, \delta(E_i - E_f)\, T_{fi} \qquad (249)$$

Using this we can express the scattering operator as

$$S = 1 + \underline{T} \qquad (250)$$

which is free from any particular representation. This not only expresses S in a compact form, but also has the advantage of leading to a simple interpretation of $\underline{T}$. Recalling equation (238), we can write

$$\underline{\Phi}^{Scatt.} = \underline{T}\,\Psi^{in} \qquad (251)$$

where $\underline{\Phi}^{Scatt.}$ is the difference between output and input states, and which can be interpreted as a scattered wave. Then $\underline{T}$ is an operator equivalent to the Green's function met with in the elementary treatment. This is not so with the S-operator, which transforms the input into the entire output.

The Lippmann - Schwinger Equations:

Having studied the S-operator, we turn our attention to the functions Ψ^{in} and Ψ^{out}, and we shall see how they enable us to obtain an explicit representation for S or T. We use a time-independent approach, and so we assume the existence of a

Hamiltonian H which governs our problem. This Hamiltonian will possess, in general both a discrete as well as a continuous spectrum of eigenvalues E and corresponding eigenfunctions Ψ :

$$H\Psi = E\Psi \tag{252}$$

We next make another important assumption, namely, that the Hamiltonian can be split into an unperturbed part H^{o} and a perturbing part H' :

$$H = H^{o} + H' \tag{253}$$

The first part H^{o} will also have a set of discrete as well as continuous eigenvalues. Now we can always adjust an energy scale so as to make the continuum start at $E = 0$, so that for the continuous spectrum $E > 0$, and for the bound states $E < 0$. In our case, we further assume that both the energy scales corresponding to the eigenvalues of H and H^{o} coincide, in other words, the continuum in both cases begins at $E = 0$. This means essentially that when the perturbation H' is switched on, the energies in the continuum states are not changed. Then for every state Ψ_a in the continuous spectrum of H , there corresponds a state Φ_a in the continuous spectrum of H^{o} , having the same energy E_a :

$$H\Psi_a = E_a\Psi_a \tag{254a}$$

$$H^{\circ}\Phi_a = E_a\Phi_a \tag{254b}$$

This one-to-one correspondence does not, of course, exist among the discrete eigenstates. If H^{o} possesses discrete eigenvalues, the perturbation will in general split and shift their levels.

We tacitly assume also that there are no bound states embedded in the continuum. Such cases, which would correspond to metastable states, will have to be considered separately.

Now from equations (254) we can write a formal solution for the unknown function Ψ as:

$$\Psi_a = \Phi_a + \frac{1}{E_a - H^o} H' \Psi_a \qquad (255)$$

This is definitely a solution of the Schrodinger equation, and it may be compared to an integral equation with the coefficient of Ψ_a on the right hand side as a kernel.

Equation (255) as it stands is unsatisfactory because of the presence of singularities. To avoid this, we can redefine the operator $(E_a - H^o)^{-1}$ as the limit of either $(E_a - H^o + i\eta)^{-1}$ or $(E_a - H^o - i\eta)^{-1}$ as $\eta \to 0$. These new operators are well-defined, for, by operating with $(E_a - H^o \pm i\eta)$ on some arbitrary eigenstate Φ_b of H^o, and manipulating the result, we easily obtain

$$\frac{1}{E_a - H^o \pm i\eta} |\Phi_b\rangle = \frac{1}{E_a - E_b \pm i\eta} |\Phi_b\rangle \qquad (256)$$

Thus all the Φ_b are eigenstates of the new operators, with eigenvalues obtained by replacing H^o by E_b. This means the operators $(E_a - H^o \pm i\eta)^{-1}$ are defined in the Hilbert space spanned by the eigenkets $|\Phi_a\rangle$.

To find the meaning of these operators in the Hilbert space defined by the total Hamiltonian H, we use the fact that there is a one-to-one correspondence between Ψ_a and Φ_a. Any arbitrary state χ which is a vector in the Hilbert space

of H, can therefore be expanded as

$$\chi = \sum C_n \Phi_n$$

where C_n will be given by

$$C_n = \langle \Phi_n | \chi \rangle$$

Then

$$\frac{1}{E_a - H^\circ \pm i\eta} | \chi \rangle = \sum_n C_n \frac{1}{E_a - E_n \pm i\eta} \Phi_n$$

$$= \sum_n \frac{1}{E_a - E_n \pm i\eta} | \Phi_n \rangle \langle \Phi_n | \chi \rangle$$

so that

$$\frac{1}{E_a - H^\circ \pm i\eta} \equiv \sum_n \frac{1}{E_a - E_n \pm i\eta} | \Phi_n \rangle \langle \Phi_n | \quad (257)$$

in the Hilbert space of H. This completes the definition of the new operators.

Substituting the new operators in equation (255), we will have in general two solutions:

$$\Psi_a^+ = \Phi_a + \lim_{\eta \to 0} \frac{1}{E_a - H^\circ + i\eta} H' \Psi_a^+ \quad (258)$$

$$\Psi_a^- = \Phi_a + \lim_{\eta \to 0} \frac{1}{E_a - H^\circ - i\eta} H' \Psi_a^- \quad (259)$$

These two important equations are called the Lippmann-Schwinger equations.

In order to study the solutions $\Psi_a^\pm$ and to distinguish between them, we introduce the time variable. We form a wave packet

corresponding to either type of solution. For example, we define

$$\Psi^{+}(t) = \sum_{A} \int f_A(E_a)\, e^{-\frac{i}{\hbar} E_a t}\, \Psi_a^{+}\, dE_a \qquad (260)$$

Here $f(E_a)$ is a varying function sharply peaked at some particular energy E_b so that the wave packet is centred around the stationary state Ψ_b. The subscript A indicates some property such as angular momentum over which a summation might have to be carried out.

We define in an exactly similar way a function $\Phi(t)$. Then using equation (258) and the expansion

$$H' \Psi_a^{+} = \sum_n C_n \Phi_n^{+}$$

we can show finally that

$$\lim_{t \to -\infty} \Psi_a^{+}(t) = \Phi_a(t) \qquad (261)$$

$$\lim_{t \to +\infty} \Psi_a^{-}(t) = \Phi_a(t) + \sum_n R_n \Phi_n \qquad (262)$$

where R_n is peaked for the state Φ_b.

This result is interpreted as follows. At a time very long before the collision the wave packet is a free wave. But long after the collision, there is a new term which corresponds to a scattered wave. Since $\Psi^{+}(t)$ is centred on Ψ_b^{+}, it follows that Ψ_b^{+} or in general any Ψ^{+}, represents an incoming state. In the simplest case, Ψ^{+} contains an incident plane wave and the scattered spherical waves.

The Ψ^{-} states may be similarly treated, that is, by forming a wave-packet and studying its asymptotic forms for the

remote past and distant future. We obtain then

$$\lim_{t \to -\infty} \Psi^{-}(t) = \Phi(t) + \sum B_n \Phi_n \qquad (263)$$

$$\lim_{t \to +\infty} \Psi^{+}(t) = \Phi(t) \qquad (264)$$

Thus the Ψ^{-} states behave as free waves long after the collision. We therefore interpret them as outgoing states. In the coordinate representation they contain an outgoing unperturbed wave and an incoming scattered wave.

In arriving at the Lippmann-Schwinger equations, we have assumed that the total Hamiltonian can be split up into two parts. If this is to be avoided, then equation (258) or (259) can be recast in another form. The equation is premultiplied by H' on both sides, and then the (original) equation is iterated by substituting for $\Psi^{\pm}$, and the two resulting equations are manipulated to lead to

$$\Psi_a^{\pm} = \pm \lim_{\eta \to 0} \frac{i\eta}{E_a - H \pm i\eta} \Phi_a \qquad (265)$$

The states Φ_a can now be considered to be merely a convenient set of free states which occur long before or long after the scattering experiment. With further manipulation, equations (265) lead to

$$\Psi_a^{\pm} = \Phi_a + \lim_{\eta \to 0} \frac{1}{E_a - H \pm i\eta} H' \Phi_a \qquad (266)$$

The operator $(E_a - H \pm i\eta)^{-1}$ can be interpreted as was the operator $(E_a - H^0 \pm i\eta)^{-1}$. In fact, a similar

argument yields the relation

$$\frac{1}{E_a - H \pm i\eta} \Psi_b^{\pm} = \frac{1}{E_a - E_b \pm i\eta} \Psi_b^{\pm} \qquad (267)$$

so that the $\Psi^{\pm}$ states are eigenstates of the operators with eigenvalues given by (267).

By expanding H into the component parts, it is possible to obtain

$$\frac{1}{E_a - H \pm i\eta} = \frac{1}{E_a - H^0 \pm i\eta} + \frac{1}{E_a - H^0 \pm i\eta} H' \frac{1}{E_a - H^0 \pm i\eta}$$

which by the iterative processes gives the Born series for this operator:

$$\frac{1}{E_a - H \pm i\eta} = \frac{1}{E_a - H^0 \pm i\eta} + \frac{1}{E_a - H^0 \pm i\eta} H' \frac{1}{E_a - H^0 \pm i\eta}$$
$$+ \frac{1}{E_a - H^0 \pm i\eta} H' \frac{1}{E_a - H^0 \pm i\eta} H' \frac{1}{E_a - H^0 \pm i\eta}$$
$$+ \cdots\cdots\cdots$$

so that a Born series for $\Psi^{\pm}$ too may be obtained from (266):

$$\Psi_a^{\pm} = \Phi_a + \frac{1}{E_a - H^0 \pm i\eta} H' \Phi_a + \frac{1}{E_a - H^0 \pm i\eta} H' \frac{1}{E_a - H^0 \pm i\eta} H' \Phi_a + \cdots\cdots \qquad (268)$$

where the limit $\eta \to 0$ is implied.

The expression (266) is useful for deducing further properties of the $\Psi^{\pm}$ solutions. For instance we can show that they are orthonormal as follows:

$$(\Psi_a^+, \Psi_b^+) = (\Phi_a, \Phi_b) + \left(\frac{1}{E_a - H + i\eta} H' \Phi_a, \Psi_b^+ \right)$$

where the limit $\eta \to 0$ is understood. The Hermitian operator

in the prefactor of the second term can be transferred to the postfactor, so that,

$$\left(\Psi_a^+, \Psi_b^+\right) = \left(\Phi_a, \Psi_b^+\right) + \left(\Phi_a, H' \frac{1}{E_a - H - i\eta} \Psi_b^+\right)$$

$$= \left(\Phi_a, \Psi_b^+\right) + \frac{1}{E_a - E_b - i\eta} \left(\Phi_a, H' \Psi_b^+\right)$$

where the last step follows from (267). Next, expanding the postfactor in the first term and performing similar manipulations as before, we have finally,

$$\left(\Psi_a^+, \Psi_b^+\right) = \left(\Phi_a, \Phi_b\right)$$

Since the states Φ_a are taken to be orthonormal, it follows that

$$\left(\Psi_a^+, \Psi_b^+\right) = \delta_{ab} \tag{269a}$$

Using a similar argument we can also show that

$$\left(\Psi_a^-, \Psi_b^-\right) = \delta_{ab} \tag{269b}$$

Further, if the Hamiltonian H possesses bound states of negative energy, denoted by Ψ_α^B, then

$$\left(\Psi_a^\pm, \Psi_\alpha^B\right) = 0 \tag{270}$$

An important property of the $\Psi^\pm$ solutions is related to their completeness. There is a theorem which states that a Hamiltonian operator satisfying certain definite boundary conditions possesses a complete set of eigenstates. This is rigorously true for a large variety of boundary conditions, but has not yet

been proved for arbitrary conditions. However, we do make the assumption that the Ψ^{+} and Ψ_{α}^{B} states together form a complete set, that is,

$$\sum_{a} |\Psi_a^{+}\rangle\langle\Psi_a^{+}| + \sum |\Psi_\alpha^{B}\rangle\langle\Psi_\alpha^{B}| = 1 \qquad (271)$$

and so also for the Ψ^{-} and Ψ_{α}^{B} states.

Yet another scalar product occurring in calculations is

$$\left(\Phi_a, \Psi_b^{\pm}\right) = \delta_{ab} + \frac{1}{E_b - E_a \pm i\eta} T_{ab}^{\pm} \qquad (272)$$

where

$$T_{ab}^{\pm} = \left(\Phi_a, H'\Psi_b^{\pm}\right)$$

The result is obtained as before by transferring the operator. The T_{ab}^{+} function is identical with the T_{fi} mentioned earlier.

The same method can be used to establish the relation

$$\left(\Psi_\alpha^{B}, \Phi_b\right) = \frac{1}{E_\alpha - E_b}\left(\Psi_\alpha^{B}, H'\Phi_b\right) \qquad (273)$$

where the first step is to replace H' by $H - H^{o}$.

<u>S and T operators defined in terms of $\Psi^{\pm}$</u>:

Let us return to equation (238) and project it on a particular state $|\, f >$ belonging to a set of eigenkets of a maximal set of observables. Using the completeness condition in the form

$$\sum_{n} |\, n\rangle\langle\, n| = 1,$$

we have

$$\langle f|\Psi^{out}\rangle = \sum \langle f|S|n\rangle\langle n|\Psi^{in}\rangle$$

Equations (239) show that the left-hand side is a particular

outgoing state corresponding to the label f, while on the right hand side the term $\langle n | \Psi^{in} \rangle$ is a particular ingoing state corresponding to n. Hence

$$\Psi_f^- = \sum_n S_{fn} \Psi_n^+ \tag{274}$$

If we take the scalar product of the above equation with some particular Ψ_i^+ then, using (269a), we have, but for a phase factor, in any representation

$$S_{fi} = (\Psi_f^- , \Psi_i^+) \tag{275}$$

Thus the full solutions of the Lippmann-Schwinger equations define the elements of the S-matrix. These states are determined by the full Hamiltonian, and therefore, in principle we can define the S-matrix without taking recourse to splitting H into unperturbed and perturbed parts. Of course, in practice this may not be possible.

In passing we may note that besides $\langle \Phi_f | S | \Phi_i \rangle$,

$$\langle \Psi_f^+ | \bar{S} | \Psi_i^+ \rangle \quad \text{or} \quad \langle \Psi_f^- | \bar{S} | \Psi_i^- \rangle$$

also define an S-matrix but different from that discussed above. It is useful in the time-dependent Heisenberg approach where the operators depend on time and the states are independent of time.

The elements S_{fi} have a simple meaning. Because of the completeness relation (271) we can write

$$\Psi_f^- = \sum_a C_a \Psi_a^+ + \sum_\alpha C_\alpha \Psi_\alpha^B$$

Forming the scalar product with Ψ_i^+ and using (269a) and (270), we find that

$$C_i = (\Psi_f^-, \Psi_i^+) = S_{fi} \tag{276}$$

The coefficient C_a is interpreted as the probability amplitude for an incoming state Ψ_a^+ to be in the outgoing state Ψ_f^-. This, we find, is exactly equal to the matrix element S_{fa}.

Any particular element may be obtained explicitly by using (266). Thus if we take a general element S_{ab}, we have

$$S_{ab} = (\Psi_a^-, \Psi^+)$$

$$= (\Phi_a, \Psi_b^+) + \left(\frac{1}{E_a - H - i\eta} H' \Phi_a, \Psi_b^+\right)$$

Transferring the operators again from the pre-factor, and using (272), we have

$$S_{ab} = \delta_{ab} + \frac{1}{E_b - E_a + i\eta}(\Phi_a, H'\Psi_b^+) + \frac{1}{E_a - E_b + i\eta}(\Phi_a, H'\Psi_b^+)$$

$$= \delta_{ab} + \frac{-2i\eta}{(E_a - E_b)^2 + \eta^2}(\Phi_a, H'\Psi_b^+)$$

Using the relation

$$\lim_{\eta \to 0} \frac{\eta}{x^2 + \eta^2} = \pi \delta(x)$$

we have

$$S_{ab} = \delta_{ab} - 2\pi i \, \delta(E_a - E_b)(\Phi_a, H'\Psi_b^+) \tag{277}$$

This equation may be compared with equation (243), and therefore we write

$$T_{ab} = \left(\Phi_a , H' \Psi_b^{+} \right) \qquad (278)$$

This expression can be used for calculating the T-matrix. If the explicit form of $\Psi_b^{\pm}$ is not known, we can use the series expansion (268) and compute the matrix element to any desired degree of approximation.

An interesting relation can be obtained for the T-matrix by using the above expression. Let us multiply the Lippmann-Schwinger equation (258) for Ψ_i^{+} on the left by H', and then take its scalar product with Φ_f :

$$\left(\Phi_f , H' \Psi_i^{+} \right) = \left(\Phi_f , H' \Phi_i \right) + \left(\Phi_f , H' \frac{1}{E_a - H^0 + i\eta} H' \Psi_i^{+} \right)$$

We introduce the completeness condition

$$\sum_r \left(\Phi_r , \Phi_r \right) = 1$$

in the second term, just in front of the second H' operator. Then using (278),

$$T_{fi} = H_{fi} + \sum_r \left(\Phi_f , H' \frac{1}{E_a - H^0 + i\eta} \Phi_r \right) T_{ri}$$

$$= H'_{fi} + \sum \frac{1}{E_a - E_r + i\eta} H'_{fr} T_{ri} \qquad (279)$$

Since this equation is valid for all the indices i and f , it

may be written in terms of the operators themselves as

$$T = H' + H' \frac{1}{E_a - H^0 + i\eta} T \qquad (280)$$

Let this operator equation be applied onto some state Φ_a . If the terms are then manipulated and the limit $\eta \to 0$ finally taken, then one obtains

$$T \Phi_a = H' \Psi_a^+ \qquad (281)$$

Application to potential scattering:

The formal expressions discussed in this chapter may be applied to ordinary potential scattering to produce familiar formulae. In the coordinate representation, the Hamiltonian is specified by

$$H^0 \equiv -\frac{\hbar^2}{2m} \nabla^2$$

$$\text{and} \quad H' = V(\underline{r})$$

and the eigenvalues of the former are, assuming that there are no bound states,

$$E_k = \frac{\hbar^2 k^2}{2m}$$

Using the completeness relation for the Φ_k , the operator $(E_k - H^0 \pm i\eta)^{-1}$ in the coordinate representation can be written as

$$\langle \underline{r}' | \frac{1}{E_k - H^0 \pm i\eta} | \underline{r}'' \rangle = \sum_{k'} \frac{1}{E_k - E_{k'} \pm i\eta} \langle \underline{r}' | \Phi_{k'} \rangle \langle \Phi_{k'} | \underline{r}'' \rangle$$

$$= \sum_{k'} \frac{1}{E_k - E_{k'} \pm i\eta} e^{i \underline{k}' \cdot \underline{r}'} e^{-i \underline{k}' \cdot \underline{r}''}$$

Strictly speaking, the summation should be an integral over the continuous variable k' :

$$\langle \underline{r}' | \frac{1}{E_k - H^\circ \pm i\eta} | \underline{r}'' \rangle = \frac{2m}{\hbar^2} \frac{1}{(2\pi)^3} \int \frac{e^{i\underline{k}'\cdot(\underline{r}'-\underline{r}'')}}{k^2 - k'^2 \pm i\varepsilon} \, d^3\underline{k}$$

Here we have expressed E_k and $E_{k'}$ in terms of k and k' respectively and replaced η by $\frac{\hbar^2}{2m}\varepsilon$. The term $(1/2\pi)^3$ is required for normalising the momentum eigenfunctions. The integral is a familiar one, leading to

$$-\frac{2m}{\hbar^2} \frac{1}{4\pi} \frac{e^{\pm ik|\underline{r}'-\underline{r}''|}}{|\underline{r}'-\underline{r}''|}$$

which is, except for the factor (- 2m / $\hbar^2$) , the outgoing or incoming Green's function $G^{\pm}(\underline{r}'-\underline{r}'')$

The Lippmann-Schwinger equation can similarly be interrupted by using (257). Then

$$|\Psi_k^+\rangle = |\Phi_k\rangle + \sum_{k'} \frac{1}{E_k - E_{k'} + i\eta} |\Phi_{k'}\rangle \langle \Phi_{k'} | H' | \Psi_k^+ \rangle$$

Substituting V for H' and introducing the completeness condition in terms of the coordinate eigenstates before and after H' , the last factor becomes

$$\langle \Phi_{k'} | H' | \Psi_k^+ \rangle = \iint \langle \Phi_{k'} | \underline{r}'' \rangle \langle \underline{r}'' | V(\underline{r}) | \underline{r}' \rangle \langle \underline{r}' | \Psi_k^+ \rangle \, d^3\underline{r}' \, d^3\underline{r}''$$

$$= \iint e^{-i\underline{k}'\cdot\underline{r}''} V(\underline{r}'') \delta(\underline{r}'-\underline{r}'') \Psi_k^+(\underline{r}) \, d^3\underline{r}' \, d^3\underline{r}''$$

$$= \int e^{-i\underline{k}'\cdot\underline{r}'} V(\underline{r}') \Psi_k^+(\underline{r}') \, d^3r'$$

where $\psi_k^+(\underline{r}')$ is the ingoing state in the $\underline{r}'$ representation. Then projecting the previous equation on the $\underline{r}'$ representation, we have

$$= e^{i\underline{k}\cdot\underline{r}} + \frac{2m}{\hbar^2}\lim_{\eta\to 0}\iint \frac{e^{i\underline{k}'\cdot(\underline{r}-\underline{r}')}}{k^2-k'^2+i\varepsilon} V(\underline{r}')\psi_k^+(\underline{r}') \, d^3k' d^3\underline{r}'$$

$$= e^{i\underline{k}\cdot\underline{r}} - \frac{1}{4\pi}\int \frac{e^{ik|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|} U(\underline{r}')\psi_k^+(\underline{r}')\, d^3\underline{r}'$$

$$= e^{i\underline{k}\cdot\underline{r}} + \int G^+(\underline{r},\underline{r}')\, U(\underline{r}')\, \psi_k^+(\underline{r}')\, d^3\underline{r}'$$

where $2mV/\hbar^2$ has been denoted by U. This equation is identical to the integral equation for ψ_k^+ obtained earlier. (Ref. equation (46).)

The elements of the reaction matrix as given by $(\Phi_a, H'\psi_b^+)$ have been calculated above. Writing $e^{i\hat{\underline{k}}\cdot\underline{r}}$ for Φ_a and $\psi_k(\underline{r})$ for ψ_b^+ in the coordinate representation, we have

$$T_{\hat{\underline{k}}\underline{k}} = \int e^{-i\hat{\underline{k}}\cdot\underline{r}} V(\underline{r})\, \psi_k^+(\underline{r})\, d^3\underline{r}$$

Comparing with (47), we see that

$$T_{\hat{\underline{k}}\underline{k}} = -\frac{2\pi\hbar^2}{m} f(k, \Delta)$$

so that the scattering amplitude $f(k, \Delta)$ is now explicitly related to the T-matrix, and hence to the S-matrix.

Chapter IX.

THE S-MATRIX IN THE ANGULAR MOMENTUM REPRESENTATION

It will be shown in this chapter that the S-matrix takes on a very useful form when expressed in the angular momentum representation. It becomes a diagonal matrix with the elements simply related to phase shifts of partial waves, if the scattering is elastic. Moreover, it lends itself easily to analytic extension by the use of the Jost functions.

To begin with, let us take the Schrodinger equation for scattering in the time-independent approach:

$$\left[\nabla^2 + k^2 - U(\underline{r})\right]\psi_k(r,\theta,\varphi) = 0 \qquad (282)$$

where the term k^2 is related to the energy and $U(\underline{r})$ to the potential function. If the potential is a central one, then the solution does not depend on φ. If expanded in terms of partial waves, the solution is written,

$$\psi_k(r,\theta) = \sum_{\ell=0}^{\infty} a_\ell(k) R_{\ell,k}(r) P_\ell(\cos\theta) \qquad (283)$$

where $a_\ell(k)$ are coefficients depending on the parameter k. $R_{\ell,k}$ is the radial wave function for the ℓ^{th} partial wave, and may be replaced by $u_{\ell,k}(r)/r$ the so called reduced radial wave function. Using this and substituting (283) in (282) we have, for each ℓ, an equation for $u_{\ell k}$:

$$u''_{\ell,k}(r) + \left[k^2 - U(r) - \frac{\ell(\ell+1)}{r^2}\right] u_{\ell,k}(r) = 0 \qquad (284)$$

Since $R(r)$ must be finite at $r = 0$, the condition imposed on

$u(r)$ is that it must be zero for $r = 0$. Such a solution is called a regular solution. The constants $a_{\ell k}$ are determined for specified boundary conditions. For instance, we require a solution $\psi_k^+(r,\theta)$ which for large r contains outgoing scattered spherical waves:

$$\psi_k^+ \sim e^{i\underline{k}\cdot\underline{r}} + f^+(k,\theta)\frac{e^{ikr}}{r} \tag{285a}$$

This corresponds to what we described as an incoming state in the previous chapter. Similarly, if the asymptotic boundary condition prescribes an incoming scattered spherical wave, we have an outgoing state,

$$\psi_k^- \sim e^{i\underline{k}\cdot\underline{r}} + f^-(k,\theta)\frac{e^{-ikr}}{r} \tag{285b}$$

The coefficients corresponding to these two cases are then given by

$$a_{\ell k}^{\pm} = i^{\ell}(2\ell+1)\, e^{\pm i\delta_\ell(k)} \tag{286}$$

where $\delta_\ell(k)$ is the phase shifts for the ℓ^{th} partial wave. The total scattering amplitude functions are given by

$$f_\ell^{\pm}(k,\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\, e^{\pm i\delta_\ell(k)} \sin\delta_\ell(k)\, P_\ell(\cos\theta) \tag{287}$$

Using (286) in (283) we have

$$\psi_k^{\pm}(r,\theta) = \sum_{\ell=0}^{\infty} i^{\ell}(2\ell+1)\, e^{\pm\delta_\ell(k)}\frac{u_{\ell k}(r)}{r} P_\ell(\cos\theta) \tag{288}$$

It will be noticed that the dependence on k and on r have been separated. The function $u_{\ell k}(r)$ is the same for incoming and for outgoing states, which are now distinguished only by the phase shifts.

(If the potential is not that of a central force, then we have to use the spherical harmonics $Y_{\ell m}(\vartheta, \varphi)$:, instead of the Legendre polynomial $P_\ell(\cos\vartheta)$.)

In the angular momentum representation every state is characterized by the magnitude $|\underline{k}|$ and the angular momentum quantum number ℓ , and is equal to the corresponding form in the series (283),

$$|k,\ell\rangle^{\pm} = i^\ell (2\ell+1)\, e^{\pm i\delta_\ell(k)} P_\ell(\cos\vartheta) \frac{u_{\ell k}(r)}{r}$$

However this state is not normalised to unity. Using

$$\int_{-1}^{+1} P_\ell(\cos\vartheta) P_{\ell'}(\cos\vartheta)\, d(\cos\vartheta) = \frac{2}{2\ell+1}\delta_{\ell\ell'}$$

and

$$\int_0^\infty u_{\ell k}(r)\, u_{\ell k'}(r)\, dr = \frac{\pi}{2k^2}\,\delta(k-k')$$

we find that

$${}^{\pm}\langle k'\ell' | k\ell\rangle^{\pm} = \frac{2\pi^2}{k^2}(2\ell+1)\,\delta_{\ell\ell'}\,\delta(k-k')$$

Therefore the normalised incoming and outgoing states must be written

$$\psi^{\pm}_{k,\ell} = \frac{k}{\pi}\frac{(2\ell+1)}{[2(2\ell+1)]^{\frac{1}{2}}}\, i^\ell\, e^{\pm i\delta_\ell(k)} \frac{u_{\ell k}(r)}{r} P_\ell(\cos\vartheta) \tag{289}$$

We now calculate the elements of the S-matrix. By (275) we have

$$S_{k\ell,k'\ell'} = \left(\psi^-_{k\ell}, \psi^+_{k'\ell'}\right)$$

$$= e^{2i\delta_\ell(k)}\,\delta_{\ell\ell'}\,\delta(k-k') \tag{290}$$

where use has been made of (289). This remarkable result shows that S is diagonal in the angular momentum representation and that the eigenvalues are merely exp ($2i \times \delta_\ell(k)$). For convenience we use the notation

$$S_\ell(k) \equiv e^{2i\delta_\ell(k)} \tag{291}$$

where $S_\ell(k)$ is called the S-function for angular momentum ℓ and linear momentum k.

This expression can be written in a very general form

$$S = e^{2iD} \tag{292}$$

The D is called the phase matrix, and it is a Hermitian operator with eigenvalues equal to the phase shifts themselves. Obviously D (and S) is diagonal in the angular momentum representation.

The expression (292) shows directly that S is unitary, that is, that SS* is the unit matrix. The unitarity of the S-matrix depends in general on whether or not H^0 has bound states. If bound states occur, it means that the incoming or outgoing states at $t \to \pm \infty$ are not free waves, and the product SS* will have terms other than the unit matrix. In the present case, however, H^0 corresponds to $-\frac{\hbar^2}{2m}\nabla^2$ which has no bound states.

The relation (291) reveals an interesting property of the S-function, namely that for real k, when $\delta_\ell(k)$ is also real,

$$|S_\ell(k)| = 1 \tag{293}$$

We say that the S-function is unimodular on the real k-axis. It is possible to take a converse point of view, that is, by demanding that S be unitary because of the conservation of probability, we can deduce that the phase angles must be real.

We now refer back to the expansion of the total scattering amplitude in terms of partial wave scattering amplitudes:

$$f(k,\vartheta) = \sum_{\ell=0}^{\infty} (2\ell+1)\, f_\ell(k)\, P_\ell(\cos\vartheta) \tag{294}$$

By comparing this with equation (287) for outgoing waves, we have

$$f_\ell(k) = \frac{1}{k}\, e^{i\delta_\ell(k)} \sin\delta_\ell(k) \tag{295}$$

Using equation (291), this becomes

$$f_\ell(k) = \frac{1}{2ik}\left[S_\ell(k) - 1\right] \tag{296}$$

This is an important relationship between the scattering amplitude and S-matrix, since the analytic properties of the latter are now directly related to those of the former.

Now it can be shown that for large r,

$$e^{i\underline{k}\cdot\underline{r}} \sim \sum_{\ell=0}^{\infty} (2\ell+1)\frac{1}{2ik}\left[\frac{e^{ikr}}{r} - (-1)^\ell \frac{e^{-ikr}}{r}\right] P_\ell(\cos\vartheta) \tag{297}$$

Substituting equations (294), (296) and (297) in equation (285a), and comparing the result with (283), we obtain

$$R^{+}_{k\ell} \sim A_\ell(k)\left[\frac{e^{-ikr}}{r} - (-1)^\ell S_\ell(k)\frac{e^{ikr}}{r}\right] \tag{298}$$

where $A_\ell(k)$ is a normalization factor. This form of $R_{\ell k}$ shows that the ℓ^{th} partial wave has both an incoming and an

outgoing spherical component, and that a phase shift is introduced between them by the factor $S_\ell(k)$. If this factor is unity, the superposition of the two components would merely give a plane wave. If $S_\ell(k)$ is different from unity, this difference throws the components out of balance. When solving the Schrödinger equation, the solution was pictured as being initially a plane wave, whose components acquired phase shifts $\delta_\ell(k)$ due to the interaction with the perturbing potential. These considerations give a pictorial meaning to S_ℓ.

The solution of the scattering problem involves essentially the determination of the phase shifts and the complex amplitudes. The computation involves coupled integral equations which are difficult to solve. This difficulty is largely avoided by the use of the Jost functions.

The Jost Functions:

We consider again equation (284), and we look for a solution restricted only by the requirement that

$$\lim_{r \to \infty} F_1(k, \ell; r) = C_\ell(k)\, e^{ikr} \qquad (299)$$

where $C_\ell(k)$ is some normalization factor. Let there also be another independent solution such that

$$\lim_{r \to \infty} F_2(k, \ell; r) = C_\ell(k)\, e^{-ikr} \qquad (300)$$

Now the differential equation (284) contains the parameter k in the form k^2, so that $F_2(-k, \ell; r)$ must also be a solution, as its asymptotic

and its asymptotic behaviour will be

$$\lim_{r \to \infty} F_2(-k, \ell; r) = C_\ell(-k) e^{ikr}$$

which is the same as (299) except for a change in the normalization factor. But since with a given boundary condition two solutions are the same, we must have

$$F_2(k, \ell; r) = F_1(-k, \ell; r) \tag{301}$$

and we denote both by the same symbol $F(k, \ell; r)$ even though they may not be linearly independent. This function is thus the general solution with the property

$$\lim_{r \to \infty} F(k, \ell; r) \sim e^{-ikr} \tag{302}$$

The constant may be dropped for convenience.

It must now be observed that the solution $F(k, \ell; r)$ need not be a regular solution, that is, it need not vanish at $r = 0$. However, if we construct a linear combination

$$\frac{F(k, \ell; 0)}{F(-k, \ell; 0)} F(-k, \ell; r) - F(k, \ell; r) \tag{303}$$

then we find that this combination vanishes for $r = 0$. We can show that this is indeed a solution of (284), and we equate it to $r R^+_{\ell k}$ so as to write for the radial wave function

$$R^+_{\ell k}(r) = \frac{F_\ell(k)}{F_\ell(-k)} \frac{F(-k, \ell; r)}{r} - \frac{F(k, \ell; r)}{r} \tag{304}$$

We have introduced the Jost function $F_\ell(k)$ which is nothing but

$$F_\ell(k) \equiv F(k, \ell; 0) \tag{305}$$

Since $R^{+}_{\ell k}(r)$ as expressed above is a solution for the energy $\frac{\hbar^2 k^2}{2m}$ and is regular at $r = 0$, the only remaining criterion is the asymptotic behaviour. Using (302) we find that

$$\lim_{r\to\infty} R^{+}_{\ell k} = \frac{F_\ell(k)}{F_\ell(-k)} \frac{e^{ikr}}{r} - \frac{e^{ikr}}{r} \qquad (396)$$

Since $F_\ell(k)$ and $F_\ell(-k)$ are both solutions of the Schrödinger equation for the same energy and taken at $r = 0$, their ratio must be of magnitude unity. Therefore equation (306) may be compared with (298), and we can write, apart from a multiplicative phase constant,

$$S_\ell(k) = (-1)^\ell \frac{F_\ell(k)}{F_\ell(-k)} \qquad (307)$$

If this is true, then (304) is indeed our desired solution.

We have thus obtained a relation between the elements of the S-matrix and the Jost function. The advantage lies in the fact that only one integral equation need be solved to determine the Jost function, so that the S-function becomes much easier to compute than if we had to solve two coupled equations.

An explicit representation for Just function is obtained by first solving the equation

$$\frac{d^2}{dr^2} F(k,\ell;r) + k^2 F(k,\ell;r) = \left[U(r) + \frac{\ell(\ell+1)}{r^2}\right] F(k,\ell;r) \qquad (308)$$

obtained by manipulating (284). We use a Green's function defined by

$$G'' + k^2 G = -\delta(r) \qquad (309)$$

which has the solution

$$G = \frac{1}{2\pi} \int \frac{e^{ik'r}}{k'^2 - k^2} \, dk'$$

The principal value of the integral is taken, so that finally

$$G(r-r') = -\frac{1}{2k} \sin k(r-r')$$

Using this, and equations (308) and (309), we arrive at

$$F(k, \ell; r) = e^{-ikr} - \frac{1}{k} \int_r^\infty \sin k(r-r') \left[U(r') + \frac{\ell(\ell+1)}{r'^2} \right] F(k, \ell; r') dr' \qquad (310)$$

It is seen that as $r \to \infty$ the desired asymptotic behaviour is obtained.

We thus have an integral equation for $F(k, \ell ; r)$. Once this is solved we can substitute $r = 0$ and hence arrive at the Jost function.

To study the analytic properties of $F_\ell(k)$, it is preferable to have an integral representation of it. Thus, using integration by parts, equation (310) can be shown to lead to

$$F_\ell(k) = 1 + (-i)^\ell \int_0^\infty j_\ell(kr') U(r') F(k, \ell; r') r' dr' \qquad (311)$$

This however is not of much use for actual computation. It is only a convenient form which we can later use for analytical extension to complex values of momentum.

Using equation (310), if we calculate $F^*(k, \ell; r)$ and $F(-k, \ell ; r)$, we find that they are identical. Thus we obtain the crossing symmetry for the Jost function:

$$F_\ell^*(k) = F_\ell(-k) \qquad (312)$$

Here k is real.

If this is used together with (291) and (307), we have

$$F_\ell(k) = |F_\ell(k)| e^{i\delta_\ell(k)} e^{-i\ell\pi/2} \tag{313}$$

The factor, $\exp(-i \times \ell\pi/2)$ could be incorporated into the definition of the Jost function. Then the phase of the Jost function is simply the phase shift δ_ℓ.

The equation (307) can be used further to prove that

$$S_\ell(k) S_\ell(-k) = 1 \tag{314}$$

This is known as the reciprocity property of the S-function. This implies that

$$\delta_\ell(-k) = -\delta_\ell(k) \tag{315}$$

From (295) it follows that

$$f(-k) = f^*(k) \tag{316}$$

In view of (294) this means that

$$f(k,\vartheta) = f^*(-k,\vartheta) \tag{317}$$

Thus using the Jost functions, we have derived the crossing symmetry relations of the scattering amplitudes in a simple manner. In contrast, it was obtained in a more complicated way in the previous treatment after using a Green's function and integral representation.

Analytic Continuation of the S-matrix:

In the time-independent approach we made use of an integral representation for the scattering amplitude, and using the Green's function g and Mercer's theorem, we derived some satisfactory information. The causality approach also reflected these results. We shall now derive the same results by adopting a new, and simpler approach, that of Jost function.

The first step is to extend the Jost function to complex values of the argument. Preparatory to this the function $F(k, \ell ; r)$ is extended, and this is done by means of a theorem of Poincaré.

Let $\Omega_x(k)$ be a linear differential operator in a single variable x and containing a parameter k. Further suppose that the coefficients occurring in the operator are regular for $a < x \leq \infty$ and that k appears as an entire function. If the solution $G(x ; k)$ of

$$\Omega_x(k) G_1(x,k) = 0$$

obeys the boundary condition that it must be independent of k, then $G(x; k)$ will be an entire analytic function of k everywhere in the complex k plane, whenever $x > a$.

If (284) is now written as a differential equation for $F(k, \ell ; r)$ we notice that the coefficients indeed are regular for $r > 0$. However, for large r, the function tends to e^{-ikr} which is not independent of k. So Poincaré's theorem is not directly applicable. However we can define a new function by

$$G(k,\ell;r) = e^{ikr} F(k,\ell;r) \qquad (378)$$

For large r, we have

$$\lim_{r \to \infty} G(k, \ell; r) = 1$$

which is independent of k. The differential equation for $G(k, \ell; r)$ is obtained by substituting

$$F(k, \ell; r) = e^{-ikr} G(k, \ell; r)$$

in the differential equation for $F(k, \ell; r)$. Hence

$$G'' - 2ikG' - \left[V(r) - \frac{\ell(\ell+1)}{r^2}\right] G = 0 \qquad (319)$$

Poincaré's theorem can now be applied to this new equation. Then we arrive at the result that for $r > 0$, $G(k, \ell; r)$ is an entire function everywhere on the complex k-plane. Consequently the original function redefined as

$$F(z, \ell; r) = e^{-izr} G(z, \ell; r) \qquad (320)$$

is also regular, but only in the lower half plane, i.e., for $\mathrm{Im}\, z < 0$, because of the exponential factor.

This does not permit us to deduce the analyticity of the Jost function, for this is obtained by putting $r = 0$ in $F(k, \ell; r)$ which however can be analytically extended only if $r > 0$. Therefore we take recourse to the integral representation for $F_\ell(k)$ in equation (311). This is tentatively written down for complex z:

$$F_\ell(z) = 1 + (-i)^\ell \int_0^\infty j_\ell(zr')\, V(r')\, F(z, \ell; r')\, r'\, dr' \qquad (321)$$

We shall use the fact that the spherical Bessel function is bounded:

$$\left| j_\ell(zr) \right| \leq C\, e^{|\mathrm{Im}\, z|\, r} \left(\frac{|z|r}{1+|z|r} \right)^{\ell+1} \qquad (322)$$

Using (320) also, we have

$$\left| F_\ell(z) - 1 \right| \leq \int_0^\infty \exp\left[\left(|\mathrm{Im}\, z| + \mathrm{Im}\, z \right) r' \right] U(r') G_n(z,\ell;r) \left(\frac{|z|r'}{1+|z|r'} \right)^{\ell+1} r'\, dr' \qquad (323)$$

In the lower half plane, the exponential term becomes unity. For large r, we know that $G \to 1$, and so also the term $\left[|z|r/(1+|z|r) \right]^{\ell+1}$. Therefore the integral converges only if

$$\int_0^\infty |U(r')| r' dr' \quad \text{exists.} \qquad (324)$$

Therefore $F_\ell(z)$ is bounded everywhere for $\mathrm{Im}\, z < 0$, provided (324) holds. Next we must prove that the differential coefficient also exists. To do this we differentiate equation (321). Since the integral has been shown to be absolutely convergent, the differentiation can be taken into the integral sign.

We use the boundedness of $\frac{d}{dz} j(zr)$ from (322) and also the fact that $\frac{dG}{dz}$ must be an entire function since G is an entire function. We can thus show that $dF_\ell(z)/dz$ also exists everywhere on the lower half of the complex momentum plane. Therefore the analytic extension (321) is valid for $\mathrm{Im}\, z < 0$.

The extension to the upper half plane is hampered by the presence of the term $\exp\left[(|\mathrm{Im}\, z| + \mathrm{Im}\, z) r' \right]$ which for $\mathrm{Im}\, z > 0$ becomes just $\exp\left[(2\,\mathrm{Im}\, z)\, r' \right]$. However, this

difficulty can be overcome if we impose a further restriction on the potential, that is by demanding that

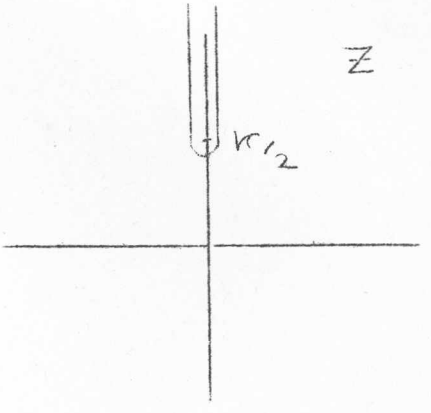
$$|U(r)| < e^{-\kappa r}, \quad r \to \infty \qquad (325)$$

where κ need only be greater than zero. In other words, the potential must decrease faster than any exponential. Another way of expressing this condition is that

$$\int_0^\infty |U(r')| r' e^{\kappa r} dr' \text{ exists} \qquad (326)$$

Under this condition the integral in (323) will converge as also will the expression for the differential coefficient of $F_\ell(z)$. Therefore $F_\ell(z)$ given by (321) is analytic in the upper half plane also, provided the more stringent condition (326) holds.

If κ is some fixed number instead of being any positive number, then the integral in (323) will converge only if



$$\text{Im } z < \kappa/2$$

and this is the range of validity of (326). However we can introduce a branch cut as shown in the figure from $i\kappa/2$ to $i\infty$.

Then the Jost function defined by (326) is analytic everhwyere in the cut z-plane.

We are in a position to extend other quantities to values of the complex argument. From(307) we can write

$$S_\ell(z) = (-1)^\ell \frac{F_\ell(z)}{F_\ell(-z)} \qquad (327)$$

Using (296), it follows that

$$f_\ell(z) = \frac{1}{2iz}\left[S_\ell(z) - 1\right] \tag{328}$$

The expression of the S-function as a ratio of two complex functions is equivalent to the N/D method which was used in Chapter V for studying the scattering amplitude. In the present case, however, the ratio occurs quite naturally, whereas in the previous case such a form had to be assumed.

Next we note the properties of the Bessel function

$$j_\ell^*(z^*) = j_\ell(z)$$

$$j_\ell(-z) = (-1)^\ell j_\ell(z)$$

and similar properties of the sine function. Then we can prove that

$$F^*(z^*, \ell; r) = F(-z, \ell; r) \tag{329}$$

and

$$F_\ell^*(z^*) = F_\ell(-z) \tag{330}$$

by calculating both sides of the equations from the respective integral equation, or integral representation, and showing that they are equal.

The reciprocity property of the S-function is valid for complex argumenta also

$$S_\ell(z)\, S_\ell(-z) = 1 \tag{331}$$

This follows from (327). It also follows that analogous to the unitary relation $S_\ell(k)\, S_\ell^*(k) = 1$, we now have

$$S_\ell(z)\, S_\ell^*(z^*) = 1 \qquad (332)$$

These are some of the properties that follow directly from the use of Jost functions.

The Poles of the S-function:

We next study the analytic behaviour of the S-function. The Jost functions have been proved to be regular in entire complex plane when the potential vanishes faster than any exponential. It may have zeros however, and whenever $F_\ell(-z)$ is zero the S-function will have a pole at that point z.

We can show that all poles occurring in the upper half plane lie only on the imaginary axis. Consider in general some point z_0 in the upper half plane ($\mathrm{Im}\, z_0 > 0$) such that $F_\ell(-z_0) = 0$. Then let us examine the function:

$$u_{\ell, z_0}(r) \equiv F(-z_0, \ell; r)$$

The right hand side is a solution of the radial Schrödinger wave equation (284), and its asymptotic behaviour for large r is $e^{iz_0 r}$ which in this case vanishes since $\mathrm{Im}\, z_0 > 0$. At $r = 0$,

$$F(-z_0, \ell; r) \equiv F_\ell(-z_0) = 0$$

so that ultimately $u_{\ell, z_0}(r)$ is also a regular solution. Therefore it satisfies the equation:

$$u_{\ell,z_0}'' + \left[z_0^2 - U(r) - \frac{\ell(\ell+1)}{r^2} \right] u_{\ell,z_0} = 0 \qquad (333a)$$

The complex conjugate of this equation is

$$u_{\ell,z_0}^{\times\,\prime\prime} + \left[z_0^{2\,\times} - U(r) - \frac{\ell(\ell+1)}{r^2} \right] u_{\ell z_0}^{\times} = 0 \qquad (333b)$$

Multiplying (333a) by $u_{\ell z_0}^{\times}$ and (333b) by $u_{\ell z_0}$ and subtracting one from the other, and then integrating the result over r, we have

$$\int_0^\infty \frac{d}{dr}\left(u' u^{\times} - u'^{\times} u \right) dr = \left(z_0^{2\,\times} - z_0^2 \right) \int_0^\infty |u|^2 \, dr$$

The left hand side of this equation vanishes since $u_{\ell z_0}(r)$ vanishes at both $r = \infty$ and $r = 0$. On the right hand side, the integrand is a positive definite quantity, so that the integral is non-zero.

Therefore $$z_0^{2\,\times} = z_0^2$$

which implies that $$g_m z_0^2 = 0$$

Since Im $z > 0$ it follows that

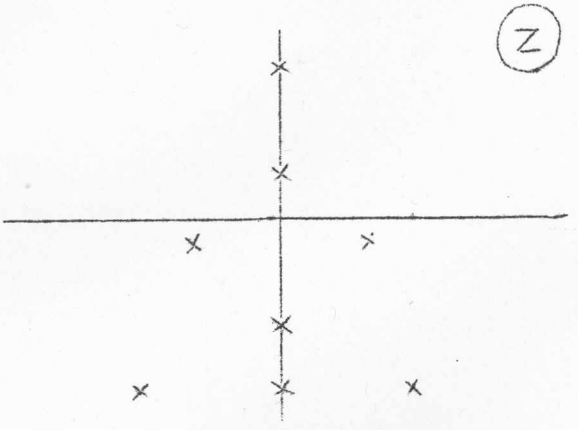
$$\text{Re } z_0 = 0$$

Therefore all poles of the S-function $S_\ell(z)$ in the upper half-plane lie on the imaginary axis.

We may here remark on the usefulness of the Schrödinger equation in obtaining the analytic properties in potential

scattering. Previously it was used indirectly to deduce the nature of the poles of the scattering amplitude from the Green's function. Without the Schrödinger equation one cannot go very far, as revealed in the causality approach.

The above argument gives no information about the poles in the lower half plane. At the most we can use the relation (330), which shows that poles must be symmetrical about the imaginary axis. Therefore on the lower half-plane, poles occur either on the imaginary axis itself or symmetrically about it.



The poles on the real axis must be treated separately, and it will be shown that there can only be one such pole, which lies at the origin. Let k_0 be some point on the real axis such that $F_\ell(k_0) = 0$. If we construct a function

$$u_{\ell,k_0}(r) = F(k_0,\ell;r) - F(-k_0,\ell;r)$$

then this function will be a regular solution, i.e., it vanishes at $r = 0$ by using (312). Then by virtue of (302) the asymptotic behaviour of the function, $u_{\ell,z_0}(r)$ is

$$u_{\ell,z_0}(r) \sim -2i \sin k_0 r$$

Also

$$u'_{\ell,k_0}(r) \sim -2ik_0 \cos k_0 r$$

Similarly we can define another function

$$V_{\ell,k_0}(r) = F(k_0,\ell;r) + F(-k_0,\ell;r)$$

This is also a regular solution and its asymptotic behaviour is

$$V_{\ell,k_0}(r) \sim 2\cos k_0 r$$

$$V'_{\ell,k_0}(r) \sim -2k_0 \sin k_0 r$$

Both u_{ℓ,k_0} and v^{x}_{ℓ,k_0} will satisfy the Schrödinger equations

$$u''_{\ell,k_0}(r) + \left[k_0^2 - U(r) - \frac{\ell(\ell+1)}{r^2}\right] u_{\ell k_0}(r) = 0$$

$$v''^{x}_{\ell,k_0}(r) + \left[k_0^2 - U(r) - \frac{\ell(\ell+1)}{r^2}\right] v^{x}_{\ell,k_0}(r) = 0$$

The first is multiplied by v^{x}_{ℓ,k_0} and the latter by u_{ℓ,k_0} and one is subtracted from the other. We have then

$$\frac{d}{dr}\left(u'v^{x} - uv'^{x}\right) = 0$$

This equation is integrated over r from zero to ∞. Substituting the above expressions for $u_{\ell k}, u'_{\ell k}$, etc., we arrive at

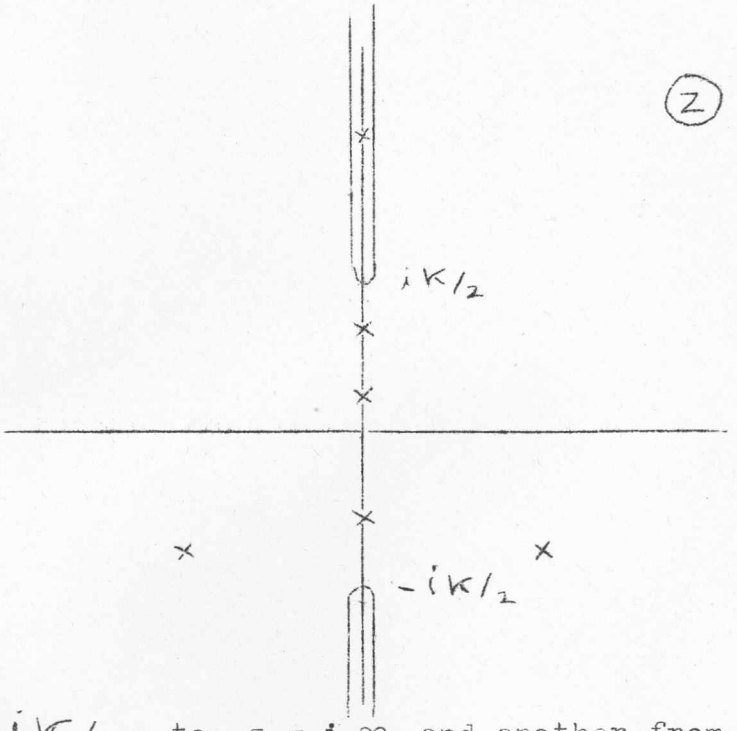
$$-2ik_0 = 0$$

or

$$k_0 = 0$$

Therefore the only pole on the real axis if there is one at all,

We have discussed the case when the potential vanishes faster than any exponential. However, if in (325) the value of κ is fixed, then there will be a cut on the imaginary axis for the Jost function. Correspondingly, there will be two cuts for the S-function, one



from $z = i\kappa/2$ to $z = i\infty$ and another from $z = -i\kappa/2$ to $z = -i\infty$. This situation may be compared to the previous one concerning the poles of the scattering amplitude. It will be recalled that there were no branch cuts arising for the total scattering amplitude $f(k, \vartheta)$. But in the case of the partial wave amplitudes $f_\ell(k)$, cuts arose because of the analytic properties of the Legendre polynomial. This is analogous to the present case since the S-function is directly related to the $f_\ell(k)$ through (296). Thus the use of Jost functions has again facilitated the discussion of analytic properties.

Next we study the properties of $S_\ell(z)$ for large z. Using the integral equation for $F(z, \ell ; r)$

$$F(z,\ell;r) = e^{-izr} - \frac{1}{z}\int_r^\infty \sin z(r-r')\left[U(r') + \frac{\ell(\ell+1)}{r'^2}\right] F(z,\ell;r')\, dr'$$

where the integral on r.h.s. is absolutely convergent, and assuming that the potential satisfies the weaker condition (324) we can show that

$$F(z, \ell ; r) \to 1 \quad \text{as} \quad |z| \to \infty, \quad \text{for} \quad \text{Im } z \leqslant 0$$

where r is arbitrary. The Jost function is a special case of this, and so it also has the same asymptotic behaviour

$$F_\ell(z) \to 1 , \quad |z| \to \infty \qquad (334)$$

If the potential is restricted by the condition that it must fall off faster than any exponential, then the Jost function is regular everywhere, and the above behaviour is true for every direction of z. If, however, the restriction is not so strong and if we have a cut on the imaginary axis, then (334) is true everywhere except along the direction of the cut. As a consequence of (327), it follows that

$$|S_\ell(z)| \to 1 , \quad |z| \to \infty \qquad (335)$$

This again is true for all directions except in those of the cuts, if any. Using this, we can immediately derive a once-subtracted dispersion relation for $S_\ell(z)$ or for the partial wave scattering amplitude $f_\ell(z)$.

Interpretation of the Poles of the S-function:

We shall next see how the poles of the S-function are to be interpreted physically. The poles on the positive imaginary axis will be seen to correspond to bound states.

It was shown earlier that all poles in the upper half plane must lie on the imaginary axis. If one such pole is $i\,|\varepsilon|$ then the corresponding energy is $-\hbar^2|\varepsilon|^2/2m$ and since this is negative, the pole ought to correspond to a bound state. This must be cheched by examining the asymptotic behaviour of the wave function.

To do this, we first take a point on the negative half of the imaginary axis $z_0 = -i\,|\varepsilon|$ and we substitute it in the regular solution of the Schrodinger equation

$$R_{\ell z}(r) = \frac{Fe(z)}{Fe(-z)}\,\frac{F(-z,\ell;r)}{r} - \frac{F(z,\ell;r)}{r} \qquad (336)$$

When r becomes very large, this behaves as

$$R_{\ell z_0}(r) \sim \frac{Fe(-i|\varepsilon|)}{Fe(i|\varepsilon|)}\,\frac{e^{|\varepsilon| r}}{r} - \frac{e^{-i|\varepsilon| r}}{r} \qquad (337)$$

This cannot be a physically meaningful solution unless the first term vanishes, i.e., we must have

$$F_\ell\,(-i\,|\varepsilon|) = 0\,.$$

This means that if we are to have a bound state with the energy negative $(= -\hbar^2|\varepsilon|^2/2m)$ then the Jost function must have a zero on the negative imaginary axis. This corresponds to a pole of the S-function in the positive imaginary axis, at $+i\,|\varepsilon|$, or because of (331) a zero at $-i\,|\varepsilon|$.

It is possible for a bound state to occur without causing a pole in the S-function. This happens when $F_\ell(-i|\epsilon|)$ and also $F_\ell(i|\epsilon|)$ are both zero. The ratio

$$S_\ell(i|\epsilon|) = (-1)^\ell \frac{F_\ell(i|\epsilon|)}{F_\ell(-i|\epsilon|)}$$

may then be finite. This is however a rare coincidence.

The above discussion on poles is strictly true only when there are no cuts in the z-plane. When the potential does not vanish faster than some exponential, then cuts will be introduced and the Jost functions will not be regular on the cuts. In such a case a pole in $S_\ell(z)$ may occur not because $F_\ell(-i|\epsilon|)$ is zero, but because $F_\ell(i|\epsilon|)$ is infinite, where $|\epsilon| > \kappa/2$. The corresponding zero in the negative imaginary axis is then called a redundant zero. Such zeros do not correspond to bound states, because for those values the radial wave function is identically zero for all r. In other words the wave simply does not exist.

To discuss poles of $S_\ell(z)$ on the negative imaginary axis, consider a point $i|\epsilon'|$ on the positive imaginary axis such that $F_\ell(i|\epsilon'|) = 0$. This gives rise to a pole of the S-function on the negative imaginary axis. The energy corresponding to this pole is $-\hbar^2|\epsilon|^2/2m$ but even though it is negative it does not correspond to a bound state. This is seen from (336), which indicates that the wave function associated with such a pole is not normalisable. However, such states are known as virtual bound states or anti-bound states and they

influence the scattering amplitude if the poles are near the origin. Then they act very much like zero-energy bound states. Actually, this type of behaviour with large scattering amplitude and small scattering length is common to all poles near the origin, whether they are on the positive part or the negative part of the imaginary axis.

The complex poles now remain to be explained. Let there be a point in the upper half plane $z_o = k + i\beta$ $(\beta > 0)$, such that $F_\ell (k + i\beta) = 0$. Then $S_\ell(z)$ will have a pole at $-k - i\beta$ below the real axis. The radial part of the wave function is given by (336) as

$$R_{\ell z_o} \doteq - \frac{F(k+i\beta, \ell; r)}{r}$$

For large r the asymptotic behaviour is

$$R_{\ell z_o} \sim - \frac{e^{-ikr}}{r} e^{\beta r} \qquad (338)$$

The energy corresponding to this state is

$$E = \frac{\hbar^2}{2m}\left[(k^2-\beta^2) + 2ik\beta\right] \qquad (339)$$

Introducing the notation

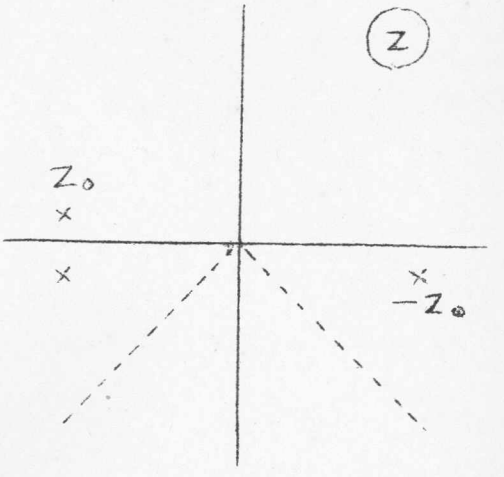
$$E_o = \frac{\hbar^2}{2m}(k^2-\beta^2) \qquad (340)$$

$$\Gamma = -\frac{\hbar^2}{2m} 2k\beta \qquad (340b)$$

the complex energy is rewritten as

$$E = E_o - i\,\Gamma/2 \qquad (341)$$

Let us first consider the case when $k < 0$. This means that z_o is in the second quadrant, and the pole is in the fourth quadrant. Then Γ is positive, while $E_o \gtrless 0$ according as $k \gtrless \beta$, that is according as the pole lies above or below the bisector in the fourth quadrant of the z-plane. We assume initially that $E_o > 0$.



The time dependent wave function is obtained by multiplying the space part by $\exp\left(-\frac{i}{\hbar} E t\right)$. For large r, the space part is (338), and therefore,

$$\Theta^{T}_{l,z}(r,t) \sim -\frac{e^{i|K|r}}{r} e^{\beta r} e^{-\frac{i}{\hbar}E_o t} e^{\frac{-\Gamma}{2\hbar}t} \qquad (342)$$

Since $E_o > 0$, this represents an outgoing state which, however, is not stable because of the exponential decay. It represents a quasi-stable state, with a mean lifetime equal to $\hbar/\Gamma$. The term $e^{\beta r}$ is of no particular consequence, except that it is necessary to conserve the number of particles. In a sense it offsets the exponential decay with time.

The poles occurring in the third quadrant may be treated in exactly the same manner. The difference now is that

k is positive, and this makes Γ negative. Consequently the asymptotic form of the total wave function is

$$\Phi_{l l_z}(r,t) \sim - \frac{e^{-i|k|r}}{r} e^{\beta r} e^{-\frac{i}{\hbar} E_0 t} e^{\frac{\Gamma}{2\hbar} t} \tag{343}$$

This represents an incoming state with an exponentially increasing amplitude. Physically, this is a capture state. Once again the factor $e^{\beta r}$ ensures particle conservation.

The discussed pair of complex poles together is phenomenologically observed as a resonance.

In both the above cases, we require that $E_0 > 0$ in order to have a physical interpretation. It may happen that poles which lie below the bisectors in the third and fourth quadrants, and which correspond to $E_0 < 0$, simply do not exist, except under very spherical circumstances.

CHAPTER X.

THE S-MATRIX IN THE FRAMEWORK OF SECOND QUANTIZATION.

In this chapter we examine the S-matrix from a different angle. In our previous discussions on scattering of a particle by a localised potential we adopted the point of view of one-particle quantum mechanics. We now discuss the S-matrix formalism in the framework of second quantization. In general a one-particle state with given momentum can be viewed as a particular excitation of the quantized matter field.

To fix our ideas let us discuss the scattering process in this framework. For simplicity we consider the case of spinless bosons which do not interact with each other.

In the discussion we shall frequently use the 'in' and 'out' operator formalism introduced in Chapter VIII. In addition to the Heisenberg field operator $\psi(\underline{r},t)$ we introduce the corresponding $\psi^{in}(\underline{r},t)$ and $\psi^{out}(\underline{r},t)$ operators. It is now recalled that

$$\lim_{t \to \mp\infty} \psi^{in}_{out}(\underline{r},t) = \lim_{t \to \mp\infty} \psi^{free}(\underline{r},t) \qquad (344)$$

The free field operator satisfies the equation

$$\frac{\hbar}{i}\frac{\partial \psi^{free}}{\partial t} - \frac{\hbar^2}{2m}\nabla^2 \psi^{free} = 0 \qquad (345)$$

whereas Ψ , the true operator satisfies the equation

$$\frac{\hbar}{i}\frac{\partial}{\partial t}\Psi - \frac{\hbar^2}{2m}\nabla^2\Psi + V(\underline{r})\Psi = 0 \qquad (346)$$

where V is a given fixed external potential. This is formally taken as the field equation. Ψ satisfies the commutation relation

$$\left[\Psi(\underline{r},t), \Psi^*(\underline{r}',t)\right]_{\text{Same time}} = \delta(\underline{r}-\underline{r}') \qquad (347)$$

Also, we expand

$$\Psi(\underline{r},t) = \sum_n a_n(t)\, u_n(\underline{r})$$

where u_n are taken to be eigenstates of the one-particle Schrödinger equation. a_n and a_n^* are interpreted as the annihilation and creation operators of the field. Also there exists the energy operator $\mathcal{H}$ which is a functional of the field variables.

The 'in' and 'out' operators are introduced in the following way. Suppose O is the operator corresponding to an observable. Then in the Heisenberg picture O satisfies

$$\dot{O}(t) = \frac{i}{\hbar}\left[H, O(t)\right] \qquad (348)$$

Performing a unitary transformation on $O(t)$ and defining $O^{in}(t)$ by

$$\Omega(t)\, O(t)\, \Omega^{-1}(t) = O^{in}(t) \qquad (349)$$

we can recast (348) to become

$$\dot{O}^{in} = \frac{i}{\hbar}\left[H^{oin}, O^{in}(t)\right] \tag{350}$$

where H^o is also considered in the same picture. This defines Ω . But this procedure facilitates only a formal simplification because we cannot find the transformation operator Ω unless we know H. However even the formal simplicity has certain advantages. We can also define another unitarity transformation

$$\Omega' O \Omega'^{-1} = O^{out} \tag{351}$$

such that $$\dot{O}^{out} = \frac{i}{\hbar}\left[H^{o\,out}, O^{out}\right] \tag{351a}$$

The difference between the 'in' and 'out' operators lies in their asymptotic behaviour with respect to time,

$$\lim_{t\to-\infty,\ t\to+\infty} O^{in}_{out} = \lim_{t\to-\infty,\ t\to+\infty} O(t) \tag{352}$$

It is worth recapitulating that, though ψ^{in}_{out} satisfies the same operator field equation and commutation relations as ψ^{free} , they are not identical. This can be seen as follows:

$$\psi^{in}_{out}(\underline{r},t) = \psi^{free}(\underline{r},t) + \int_{-\infty}^{+\infty} G^{R}_{A}(t-t')\,V(\underline{r})\,\psi(\underline{r},t')\,dt' \tag{353}$$

Here $G_{\substack{R\\A}}$ is a temporal Green's function operator satisfying the equation

$$\frac{\hbar}{i}\frac{\partial}{\partial t}G_{\substack{R\\A}}(t-t') - \frac{\hbar^2}{2m}\nabla^2 G_{\substack{R\\A}}(t-t') = -\delta(t-t') \tag{354}$$

with the respective boundary conditions

$$\left.\begin{aligned} G_R(t-t') &= 0 \quad \text{if } t < t' \\ G_A(t-t') &= 0 \quad \text{if } t > t' \end{aligned}\right\} \tag{355}$$

∇^2 has no effect on $G(t-t')$. So the solution of (354) is written as

$$G(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{e^{i\alpha t}}{-\frac{\hbar^2}{2m}\nabla^2 + i\hbar\alpha}\, d\alpha \tag{356}$$

The path of integration is so chosen as to satisfy the boundary conditions (355).

The next step is to prove,

$$\lim_{t \to \mp\infty} \psi(\underline{r},t) = \lim_{t \to \mp\infty} \psi^{\substack{in\\out}}(\underline{r},t) \tag{357}$$

provided $V(\underline{r})$ vanishes faster than $1/r$ for $r \to \infty$.

To start with let us define

$$\varphi(\underline{r},t;t') = \exp\left\{-\frac{i}{\hbar}(t-t')\left(-\frac{\hbar^2\nabla^2}{2m}\right)\right\}\cdot\psi(\underline{r},t') \tag{358}$$

where $\psi(\underline{r},t)$ is the true Heisenberg field operator, satisfying (346). Before proceeding further we have to see whether the operator $\varphi(\underline{r},t,t')$ exists. We know that, if A and

B are two commuting bound operators, then

$$e^{(A+B)} = e^{A}\, e^{B}$$

Setting $A = -\frac{\hbar}{i}\frac{\partial}{\partial t}$ and $B = -V(\underline{r})$ and using (346), we arrive at

$$\varphi_1(\underline{r},t;t') = \exp\left\{(t-t')\frac{\partial}{\partial t'}\right\}\exp\left\{\frac{i}{\hbar}(t-t')V(\underline{r})\right\}\psi(\underline{r},t') \qquad (359)$$

If an operator e^{A} is to exist, A must be a bounded operator. i.e.

$$\| A\underline{\Phi} \| < c\| \underline{\Phi} \|$$

for any element $\underline{\Phi}$ of the Hilbert space on which A acts. So if $\varphi(\underline{r},t;t')$ is to exist, then $\frac{i}{\hbar}(t-t')V(\underline{r})$ must be a bounded operator. There is, however, no difficulty arising from the operator $\exp\left\{(t-t')\frac{\partial}{\partial t}\right\}$ which simply implies a translation in time. It is also seen that $|V(\underline{r})|$ is bounded if it vanishes faster than $1/r$ as $r \to \infty$. This condition is obeyed by all physically interesting potentials. Therefore the exponential operator we have defined, exists. A final substitution proves that φ satisfies the free field operator equation

$$\frac{\hbar}{i}\frac{\partial}{\partial t}\varphi - \frac{\hbar^2}{2m}\nabla^2\varphi = 0 \qquad (360)$$

For $t = t'$, φ and $\psi(\underline{r},t)$ are identical.

We now proceed to discuss the properties of the auxiliary free field φ. Let us consider the identity

$$\int_{-\infty}^{t} \frac{\partial \varphi}{\partial t'} dt' = \varphi(\underline{r},t;t) - \varphi(\underline{r},t;-\infty) \quad (361)$$

The first term on the right hand side is just $\psi(\underline{r},t)$. The second term is $\psi^{free}(\underline{r},t)$ as defined by (353). Taking the limit $t \to -\infty$ of (361), we obtain

$$\lim_{t \to -\infty} \psi(\underline{r},t) = \lim_{t \to -\infty} \psi^{free}(\underline{r},t) \quad (362)$$

But we have already mentioned that

$$\lim_{t \to -\infty} \psi^{in}(\underline{r},t) = \lim_{t \to -\infty} \psi^{free}(\underline{r},t) \quad (363)$$

and therefore

$$\lim_{t \to -\infty} \psi(\underline{r},t) = \lim_{t \to -\infty} \psi^{in}(\underline{r},t) \quad (363a)$$

In a similar fashion we prove also the result

$$\lim_{t \to \infty} \psi(\underline{r},t) = \lim_{t \to \infty} \psi^{out}(\underline{r},t) \quad (363b)$$

Thus we have established contact with the standard procedure. The utility of this approach consists in the fact that for $t \to +\infty$ and $t \to -\infty$, $\psi(\underline{r},t)$ are related to free field solutions.

The next step is to expand ψ, ψ^{in} and ψ^{out} in terms of a complete set of orthonormal functions. This procedure will enable us to obtain the annihilation and creation operators for particles with given momentum. Let us define a complete set of functions $\Phi_k(\underline{r},t)$ which satisfy the

particle free Schrödinger equation:

$$\frac{\hbar}{i}\frac{\partial \underline{\Phi}_{\underline{k}}(\underline{r},t)}{\partial t} - \frac{\hbar^2}{2m}\nabla^2 \underline{\Phi}_{\underline{k}}(\underline{r},t) = 0 \qquad (364)$$

and which are square integrable. Then we express

$$\Psi(\underline{r},t) = \sum_{\underline{k}} a_{\underline{k}}(t)\underline{\Phi}_{\underline{k}}(\underline{r},t) \qquad (365a)$$

$$\Psi^{in}(\underline{r},t) = \sum_{\underline{k}} a_{\underline{k}}^{in}\,\underline{\Phi}_{\underline{k}}(\underline{r},t) \qquad (365b)$$

$$\Psi^{out}(\underline{r},t) = \sum_{\underline{k}} a_{\underline{k}}^{out}\,\underline{\Phi}_{\underline{k}}(\underline{r},t) \qquad (366c)$$

which define the annihilation operators $a_{\underline{k}}$, $a_{\underline{k}}^{in}$, $a_{\underline{k}}^{out}$ The creation operators $a_{\underline{k}}^{*}$, $a_{\underline{k}}^{in*}$, $a_{\underline{k}}^{out*}$ are defined by the adjoints of the above equations. It is to be noted* that the coeffidents $a_{\underline{k}}^{in*}$ and $a_{\underline{k}}^{out*}$ do not depend on t. Also note that $\underline{\Phi}_{\underline{k}}(\underline{r},t)$ is a non-quantized function having the property of a classical wave packet with characteristic peaking. The operator character of Ψ is taken care of by the 'a's. It is easily verified using the commutation relations for Ψ, Ψ^{in} and Ψ^{out}, that

$$\left[a_{\underline{k}}(t), a_{\underline{k}'}^{*}(t)\right]_{\text{same time}} = \delta_{\underline{k}\,\underline{k}'} \qquad (366a)$$

$$\left[a_{\underline{k}}^{in\,out}, a_{\underline{k}'}^{in\,out\,*}\right] = \delta_{\underline{k}\,\underline{k}'} \qquad (366b)$$

In the commutation relation (366) the question of t does not at all arise for $a_{\underline{k}}^{in\,out}$ are independent of time. In fact

*This follows from the fact that Ψ^{in}_{out} and $\underline{\Phi}_{\underline{k}}(\underline{r},t)$ satisfy the same equation.

this is precisely the advantage in using $\Phi_k(\underline{r},t)$ as the base. If we used just $\Phi_k(\underline{r})$, then $a_{\underline{k}}^{in\,out}$ have to depend on time.

Let $|0\rangle$ denote the vaccuum state of the quantized matter field. Then

$$a_{\underline{k}}^{*}(t)\,|0\rangle = \Psi_{\underline{k}}(t) \tag{367a}$$

is defined as the true one-particle state with momentum $\underline{k}$. Again, $\Psi_{\underline{k}}^{+}$ denotes by definition, a one-particle 'incoming' state with momentum $\underline{k}$:

$$a_{\underline{k}}^{in\,*}\,|0\rangle = \Psi_{\underline{k}}^{+} \tag{367b}$$

and $\Psi_{\underline{k}}^{-}$ denotes a one-particle 'outgoing' state with momentum $\underline{k}$:

$$a_{\underline{k}}^{out\,*}\,|0\rangle = \Psi_{\underline{k}}^{-} \tag{367c}$$

It is also seen that

$$a_{\underline{k}}|0\rangle = a_{\underline{k}}^{in}|0\rangle = a_{\underline{k}}^{out}\,|0\rangle = 0 \tag{368}$$

or alternatively,

$$\psi(\underline{r},t)\,|0\rangle = \psi^{in}(\underline{r},t)\,|0\rangle = \psi^{out}(\underline{r},t)\,|0\rangle = 0 \tag{369}$$

A few remarks on the set $\Phi_{\underline{k}}(\underline{r},t)$ are relevant. If we identify $\Phi_{\underline{k}}(\underline{r},t)$ with simple plane waves $e^{i\underline{k}.\underline{r}}\,e^{-\frac{i}{\hbar}E_k t}$ then the particle states $\psi^{*}_{(\underline{r},t)}|0\rangle$ etc. in co-ordinate space will not be normalisable in the strict sense. Therefore $\Phi_{\underline{k}}(\underline{r},t)$ is considdred rather as a

narrow wave packet; when the states $\psi^*(\underline{r},t)|0\rangle$ become localised states. Nevertheless when we have to perform an integration of the products containing $\Phi_{\underline{k}}(\underline{r},t)$ factors, it will be permissible to go to the limit when $\Phi_{\underline{k}}$ becomes a plane wave*,

$$\Phi_{\underline{k}}(\underline{r},t) \approx e^{i\underline{k}.\underline{r}} e^{-i/\hbar E_k t} \tag{370}$$

where

$$E_k = \frac{\hbar^2 k^2}{2m}$$

Thus equipped, we proceed to the evaluation of the elements of the S-matrix. We define

$$S_{\hat{\underline{k}}\underline{k}_0} = \langle \Psi^-_{\hat{\underline{k}}} | \Psi^+_{\underline{k}_0} \rangle \tag{371}$$

as the matrix element for the transition $\underline{k}_0 \rightarrow \hat{\underline{k}}$ where $\underline{k}_0$ is the initial state and $\hat{\underline{k}}$ is the final state. We cannot straightaway assume the validity of equation (371) for we are yet to interpret $\Psi^{\pm}$. If Ψ^- and Ψ^+ are proved to have the incoming and outgoing properties of the solution of the Schrödinger equation then equation (371) and justify it in the following treatment.

Using equation (367b)

$$S_{\hat{\underline{k}}\underline{k}_0} = \langle \Psi^-_{\hat{\underline{k}}} | a^{in*}_{\underline{k}_0} | 0 \rangle \tag{372}$$

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*We can adopt "box-normalisation" procedure and speak of the existence of the integral

$$\int |\Phi_{\underline{k}}(\underline{r},t)|^2 d^3\underline{r}$$

From equation (363a) and equation (365b) it follows that

$$\lim_{t \to -\infty} a_{\underline{k}}(t) = a_{\underline{k}}^{in} \tag{373a}$$

Again from equation (20b) and equation (22c) we get

$$\lim_{t \to +\infty} a_{\underline{k}}(t) = a_{\underline{k}}^{out} \tag{373b}$$

Using equation (373a) in equation (372)

$$S_{\hat{\underline{k}}\,\underline{k}_0} = \lim_{t \to -\infty} \langle \Psi^{-}_{\hat{\underline{k}}} | a^{*}_{\underline{k}_0}(t) | 0 \rangle \tag{374}$$

We recall that (ref. equation (243)) S_{fi} was written in the form

$$S_{fi} = \delta_{fi} - 2\pi i\, \delta(E_f - E_i)\, T_{fi}$$

To throw $S_{\hat{\underline{k}}\,\underline{k}_0}$ in the above form we rewrite equation (374) as

$$S_{\hat{\underline{k}}\,\underline{k}_0} = \lim_{t \to \infty} \langle \Psi^{-}_{\hat{\underline{k}}} | a^{*}_{\underline{k}_0}(t) | 0 \rangle - \int_{-\infty}^{\infty} \frac{d}{dt} \langle \Psi^{-}_{\hat{\underline{k}}} | a^{*}_{\underline{k}_0}(t) | 0 \rangle \, dt \tag{375a}$$

Considering the first term on the right hand side of (375a),

$$\lim_{t \to \infty} \langle \Psi^{-}_{\hat{\underline{k}}} | a^{*}_{\underline{k}_0}(t) | 0 \rangle = \langle \Psi^{-}_{\hat{\underline{k}}} | a^{out}_{\underline{k}_0} | 0 \rangle \qquad \text{using eqn. (373b)}$$

$$= \langle \Psi^{-}_{\hat{\underline{k}}} | \Psi^{-}_{\underline{k}_0} \rangle \qquad \text{using eqn. (367c)}$$

$$= \delta_{\hat{\underline{k}}\,\underline{k}_0} \qquad \text{using the orthonormality of } \Psi^{-}_{\underline{k}}\text{'s}.$$

Therefore we arrive at the modified relation

$$S_{\hat{\underline{k}}\underline{k}_0} = \delta_{\hat{\underline{k}}\underline{k}_0} - \int_{-\infty}^{\infty} \frac{d}{dt} \left\langle \underset{I}{\Psi}^{-}_{\hat{\underline{k}}} \middle| a^{*}_{\underline{k}_0}(t) \middle| 0 \right\rangle dt \qquad \textbf{(375b)}$$

Let us put

$$I = \int_{-\infty}^{\infty} \frac{d}{dt} \left\langle \underset{I}{\Psi}^{-}_{\hat{\underline{k}}} \middle| a^{*}_{\underline{k}_0}(t) \middle| 0 \right\rangle$$

Now we aim at evaluating the T matrix. To this end we have to study the integral I, defined above. (Ironically enough the simplification of I consists in first complicating the expressionfor I more and more!) The Herm tian conjugate of equation (365a) is,

$$a^{*}_{\underline{k}_0} = \int \underset{I}{\Phi}_{\underline{k}_0}(\underline{r}, t)\, \psi^{*}(\underline{r}, t)\, d^3\underline{r} \qquad (376)$$

Then

$$I = \int_{\text{Space}} \int_{-\infty}^{\infty} dt \, \frac{d}{dt} \left\{ \left\langle \underset{I}{\Psi}^{-}_{\hat{\underline{k}}} \middle| \psi^{*}(\underline{r}, t) \middle| 0 \right\rangle \underset{I}{\Phi}_{\underline{k}_0}(\underline{r}, t) \right\} d^3\underline{r}$$

The $\underset{I}{\Phi}_{\underline{k}_0}(\underline{r}, t)$ is a C-number function which can be taken out to the right. Performing the time differentiation and using the equivalent expressions for $\frac{d}{dt} \underset{I}{\Phi}_{\underline{k}}(\underline{r}, t)$ and $\frac{d}{dt} \left\langle \underset{I}{\Psi}^{-}_{\underline{k}} \middle| \psi^{*}(\underline{r}, t) \middle| 0 \right\rangle$ from equations (364) and (346) respectively we arrive at

$$I = \frac{i}{\hbar} \int_{-\infty}^{\infty} \left\{ \left\langle \underset{I}{\Psi}^{-}_{\hat{\underline{k}}} \middle| \psi^{*} \middle| 0 \right\rangle \frac{\hbar^2}{2m} \nabla^2 \underset{I}{\Phi}_{\underline{k}_0} - \underset{I}{\Phi}_{\underline{k}_0} \frac{\hbar^2}{2m} \nabla^2 \left\langle \underset{I}{\Psi}^{-}_{\hat{\underline{k}}} \middle| \psi^{*} \middle| 0 \right\rangle \right.$$

$$\left. + \underset{I}{\Phi}_{\underline{k}_0} V(\underline{r}) \left\langle \underset{I}{\Psi}^{-}_{\hat{\underline{k}}} \middle| \psi^{*} \middle| 0 \right\rangle \right\} dt\, d^3\underline{r} \qquad (377)$$

If ψ^* and $\nabla\psi^*$ vanish sufficiently fast as $r \to \infty$, we have, from Green's integral formula

$$\int\left(\psi^* \nabla^2 \underline{\Phi}_{\underline{k}_0} - \underline{\Phi}_{\underline{k}_0} \nabla^2 \psi^*\right) d^3\underline{r} = \int_{\text{surface}} \left(\psi^* \nabla \underline{\Phi}_{\underline{k}_0} - \underline{\Phi}_{\underline{k}_0} \nabla \psi^*\right) \cdot d\underline{A}$$

$\to 0$

Therefore equation (377) reduces to

$$\underline{I} = \frac{i}{\hbar} \int_{-\infty}^{\infty} V(\underline{r}) \langle \underline{\Psi}_{\hat{\underline{k}}} | \psi^* | 0 \rangle \, \underline{\Phi}_{\underline{k}_0}(\underline{r}, t) \, dt \, d^3\underline{r} \qquad (378)$$

To 'reduce' equation (378) further we recall that ψ^* is an operator in the Heisenberg picture,

$$\psi^*(\underline{r}, t) = e^{\frac{i}{\hbar} t \mathcal{H}} \psi^*(\underline{r}, 0) \, e^{-\frac{i}{\hbar} t \mathcal{H}} , \qquad (379)$$

$\mathcal{H}$ being the Hamiltonian operator of the matter field. For the ground state we have

$$\mathcal{H} |0\rangle = 0 \qquad (380)$$

This means that the eigenvalue of the total Hamiltonian corresponding to the vaccum state is 0 . Therefore

$$e^{-\frac{i}{\hbar} t \mathcal{H}} |0\rangle = |0\rangle \qquad (381)$$

Noting that $\underline{\Psi}_{\hat{\underline{k}}}$ is also an eigenstate of the Hamiltonian $\mathcal{H}$

$$\mathcal{H} \underline{\Psi}_{\hat{\underline{k}}} = E_{\hat{\underline{k}}} \underline{\Psi}_{\hat{\underline{k}}} \qquad (382)$$

we have

$$\langle \Psi^{-}_{\hat{k}} | \, e^{\frac{i}{\hbar} t \mathcal{H}} = \langle \Psi^{-}_{\hat{k}} | \, e^{\frac{i}{\hbar} E_{k'} t} \qquad (383)$$

Therefore

$$\langle \Psi^{-}_{\hat{k}} | \, \psi^{*}(\underline{r},t) | 0 \rangle = e^{\frac{i}{\hbar} E_{k'} t} \langle \Psi^{-}_{\hat{k}} | \, \psi^{*}(\underline{r},0) | 0 \rangle \qquad (384)$$

In the expression for I we replace $\Phi^{+}_{\underline{k}_0}(\underline{r},t)$ by $e^{i \underline{k}_0 \cdot \underline{r}} e^{-\frac{i}{\hbar} E_k t}$

This is allowed because we now integrate over all space and time.

Therefore,

$$I = \frac{i}{\hbar} \int\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(E_{k'} - E_k)t} V(\underline{r}) \langle \Psi^{-}_{\hat{k}} | \, \psi^{*}(\underline{r},0) | 0 \rangle e^{i \underline{k}_0 \cdot \underline{r}} \, dt \, d^3\underline{r}$$

After effecting the time integration, we have

$$I = 2\pi i \, \delta(E_{k'} - E_k) \int V(\underline{r}) \langle \Psi^{-}_{\hat{k}} | \, \psi^{*}(\underline{r},0) | 0 \rangle e^{i \underline{k}_0 \cdot \underline{r}} \, d^3\underline{r}$$

Using the above result equation (375b) reduces to

$$S_{\hat{k}\,\underline{k}_0} = \delta_{\hat{k}\,\underline{k}_0} - 2\pi i \, \delta(E_{k'} - E_k) \int V(\underline{r}) \langle \Psi^{-}_{\hat{k}} | \, \psi^{*}(\underline{r},0) | 0 \rangle e^{i \underline{k}_0 \cdot \underline{r}} \, d^3\underline{r} \qquad (385)$$

Comparing equation (385) with the standard relation

$$S_{fi} = \delta_{fi} - 2\pi i \, \delta(E_f - E_i) \, T_{fi}$$

we immediately see that

$$T_{\hat{k}\underline{k}_0} = \int \langle \bar{\psi}_{\hat{k}}^{-} | \psi^{*}(\underline{r},0) | 0 \rangle V(\underline{r}) e^{i\underline{k}_0 \cdot \underline{r}} d^3\underline{r}$$

Here we note that ψ^{*} which is time-independent is the stationary operator in coordinate space. Recognising the possibility of the superposition of different plane waves, the space part of $\Phi_{\underline{k}_0}(\underline{r},t)$ is written as $\Phi_{\underline{k}_0}(\underline{r})$ instead of $e^{i\underline{k}_0 \cdot \underline{r}}$ in the expression for $T_{\hat{k}\underline{k}_0}$. Therefore the more general expression for $T_{\hat{k}\underline{k}_0}$ is

$$T_{\hat{k}\underline{k}_0} = \int \langle \bar{\psi}_{\hat{k}}^{-} | \psi^{*}(\underline{r},0) | 0 \rangle V(\underline{r}) \Phi_{\underline{k}_0}(\underline{r}) d^3\underline{r} \quad (386)$$

Let us introduce the abbreviation

$$M^{x} = \bar{\psi}_{\hat{k}}^{-}(\underline{r}) = \langle 0 | \psi(\underline{r},0) | \bar{\psi}_{\hat{k}}^{-} \rangle \quad (387)$$

Then

$$T_{\hat{k}\underline{k}_0} = \int \bar{\psi}_{\hat{k}}^{-x}(\underline{r}) V(\underline{r}) \Phi_{\underline{k}_0}(\underline{r}) d^3\underline{r}$$

$$= \left(\bar{\psi}_{\hat{k}}^{-}, V(\underline{r}) \Phi_{\underline{k}_0} \right) \quad (388)$$

In fact the choice of the notation $\bar{\psi}_{\hat{k}}^{-}(\underline{r})$ suggests that $\langle 0 | \psi(\underline{r},0) | \bar{\psi}_{\hat{k}}^{-} \rangle$ is the conventional one-particle wave function in the configuration space. Therefore our next step consist in proving that $\bar{\psi}_{\hat{k}}^{-}(\underline{r})$ is indeed the one-particle outgoing state function in the configuration space of the customary one-particle quantum mechanics.

However, before proceeding to the proof proper it is worthwhile summarising the notations employed so far.

$\Psi(\underline{r},t)$ Field operators defined in the Hilbert space of a many -particle system. They form an uncountable continuum.

$\tilde{\Psi}_{\underline{k}}(\underline{r},t) = a^{*}_{\underline{k}}(t)|0\rangle$ one-particle momentum-space states.

$\Psi^{*}(\underline{r},t)|0\rangle$ The one particle Fock states. Arises out of the superposition of all momentum states. Though they do not have fixed momenta, are yet localisable.

$M(\underline{r},t)$ Wave functions in configuration space satisfying one-particle Schrödinger equation with a sharp momentum.

$\Phi_{\underline{k}}(\underline{r},t)$ Free nonquantized wave which formally belongs to energy corresponding to $\underline{k}$. This is not identical with M .

Now we proceed to prove that the matrix element

$$M = \langle \tilde{\Psi}^{-}_{\underline{k}} | \Psi^{*}(\underline{r},0)|0\rangle = \left(\tilde{\Psi}^{-}_{\underline{k}}(\underline{r})\right)^{*} \qquad (389)$$

satisfies the Lippmann-Schwinger equation

$$\tilde{\Psi}^{-}_{f} = \Phi_{f} + \lim_{\eta\to 0} \frac{1}{E - H^{0} - i\eta} H' \tilde{\Psi}^{-}_{f} \qquad (390)$$

In coordinate representation we have

$$H^{0} = -\frac{\hbar^{2}}{2m}\nabla^{2} \qquad (391)$$

and $H' = V(\underline{r})$

Writing $M = \langle \Psi_{\underline{k}}^{-} | \psi^{*}(\underline{r},0) | 0 \rangle$

we have $M = \langle 0 | a_{\underline{k}}^{out} \psi^{*}(\underline{r},0) | 0 \rangle$, using eqnn. (367c)

Again using equation (373b),

$$M = \lim_{t \to \infty} \langle 0 | a_{\underline{k}}(t) \psi^{*}(\underline{r},0) | 0 \rangle \qquad (392)$$

From equation (365a) we have [also refer equation (376)],

$$a_{\underline{k}}(t) = \int \overset{\leftrightarrow}{\Phi}_{\underline{k}}^{*}(\underline{r}',t)\, \psi(\underline{r}'t)\, d^3\underline{r}$$

Therefore equation (392) reduces to

$$M = \lim_{t \to \infty} \int \overset{\leftrightarrow}{\Phi}_{\underline{k}}(\underline{r}',t) \langle 0 | \psi(\underline{r}',t)\, \psi^{*}(\underline{r},0) | 0 \rangle\, d^3\underline{r}' \qquad (393)$$

As t is always greater than 0 in equation (393) we can replace $\psi(\underline{r}',t)\,\psi^{*}(\underline{r},0)$ by $P\left(\psi(\underline{r}',t)\,\psi^{*}(\underline{r},0)\right)$ where P is Dysons' chronological ordering operator. Employing the same trick as was used to arrive at equation (375a), we get

$$M = \lim_{t \to -\infty} \int \overset{\leftrightarrow}{\Phi}_{\underline{k}}^{*}(\underline{r}',t) \langle 0 | P\left(\psi(\underline{r}',t)\,\psi^{*}(\underline{r},0)\right) | 0 \rangle\, d^3\underline{r}'$$

$$+ \int_{-\infty}^{\infty} \int \frac{\partial}{\partial t} \left\{ \overset{\leftrightarrow}{\Phi}_{\underline{k}}^{*}(\underline{r}',t) \langle 0 | P\left(\psi(\underline{r}',t)\,\psi^{*}(\underline{r}',0)\right) | 0 \rangle \right\} dt\, d^3\underline{r} \qquad (394)$$

We now show that the first term on the right vaniehs. For,

$$\lim_{t\to-\infty}\langle 0|P(\psi(\underline{r}',t)\psi^*(\underline{r}',0)|0\rangle$$

$$=\lim_{t\to-\infty}\langle 0|\psi^*(\underline{r},0)\psi(\underline{r}',t)|0\rangle$$

$$=\lim_{t\to-\infty}\langle 0|\psi^*(\underline{r},0)\psi^{in}(\underline{r}',t)|0\rangle$$

$$=0,$$

using equation (363a) and $\psi^{in}(\underline{r},t)|0\rangle=0$. We note the following sailent points.

1) $\psi(\underline{r}',t)|0\rangle=0$ for no interaction between particles and 2) $\psi(r',t)|0\rangle\neq 0$ if there were interactions present. But even then one would have $\psi^{in}(\underline{r}',t)|0\rangle=0$. This is the reason why we introduced ψ^{in} in the above manipulation, although for our present purposes this was not necessary.

Considering the second term in equation (394), we perform the time-differentiation in an elementary way, use the complex conjugate of equation (346), employ Green's integral formula and obtain

$$M=\int\int_{-\infty}^{\infty}\Phi_{\underline{k}}^{in\,*}(\underline{r}',t)\left\{\frac{\partial}{\partial t}-\frac{i\hbar^2}{\hbar 2m}\nabla_{\underline{r}'}^2\right\}\langle 0|P(\psi(\underline{r}',t)\psi^*(\underline{r},0)|0\rangle \quad (395)$$
$$dt\,d^3\underline{r}'$$

We now write the time ordered product in terms of the step function*.

$$P\left(\psi(\underline{r}';t)\psi^{*}(\underline{r},0)\right) = \psi(\underline{r}';t)\psi^{*}(\underline{r},0) - \theta(-t)\left[\psi(\underline{r}';t),\psi^{*}(\underline{r},0)\right] \quad (396)$$

It is easy to check the correctness of the identify (396) if we recall the definition of $\theta(x)$. It is a matter of simple algebra to obtain

$$\left\{\frac{\partial}{\partial t} - \frac{i}{\hbar}\frac{\hbar^2}{2m}\nabla^2_{\underline{r}'}\right\}P\left(\psi(\underline{r}';t)\psi^{*}(\underline{r},0)\right)$$

$$= -\frac{i}{\hbar}V(\underline{r}')\,\psi(\underline{r}';t)\,\psi^{*}(\underline{r},0)$$

$$+ \delta(t)\left[\psi(\underline{r}';t),\psi^{*}(\underline{r},0)\right]$$

$$+ \theta(-t)\,\frac{i}{\hbar}V(\underline{r}')\left[\psi(\underline{r}';t),\psi^{*}(\underline{r},0)\right]$$

$$= \delta(t)\left[\psi(\underline{r}';t),\psi^{*}(\underline{r},0)\right]$$

$$- \frac{i}{\hbar}V(\underline{r}')\,P\left(\psi(\underline{r}';t)\,\psi^{*}(\underline{r},0)\right)$$

Here use has been made of equation (396), the complex conjugate of equation (346) and the formula

$$\frac{d}{dt}\theta(-t) = -\delta(t)$$

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*More generally,

$$P\left(A(t_1)B(t_2)\right) = A(t_1)B(t_2) - \theta(t_2-t_1)\left[A(t_1),B(t_2)\right]$$

The entire expression (396) has to be sandwiched between the states $\langle 0|$ and $|0\rangle$ and substituted in equation (395). The time integration can be performed in a trivial way using the $\delta(t)$ and it leads to an integrand (with respect to space) involving the commutator $\left[\psi(\underline{r}',0), \psi^*(\underline{r}',0)\right]$. This being an equal time commutator, we know that

$$\left[\psi(\underline{r}',0), \psi^*(\underline{r},0)\right] = \delta(\underline{r}'-\underline{r})$$

Therefore the space integration also becomes trivial. Finally we arrive at the following expression for M:

$$M = \Phi^{\times}_{\underline{k}}(\underline{r},0) - \frac{i}{\hbar}\int\int_{-\infty}^{\infty} \Phi^{\times}_{\underline{k}}(\underline{r}',t)\, V(\underline{r}') \langle 0|P\left(\psi(\underline{r}',t)\,\psi^{\times}(\underline{r},0)\right)|0\rangle\, dt\, d^3\underline{r}$$

7 (398)

We now digress a little to make certain important observations. Consider

$$K^+(\underline{r}-\underline{r}', t-t') \equiv -i\langle 0|P\left(\psi(\underline{r},t)\,\psi^*(\underline{r}',t')\right)|0\rangle \quad (399)$$

It can be easily verified that K^+ is the complete space-time retorded Green's function of the Schrodinger equation satisfying

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\nabla^2 - V(\underline{r})\right) K^+(\underline{r}-\underline{r}', t-t') = -\delta(\underline{r}-\underline{r}')\,\delta(t-t') \quad (400)$$

In terms of the Green's function M is then given by

$$M = \overset{I}{\Phi}_{\underline{k}}^{\times}(\underline{r},0) + \frac{1}{\hbar}\iint_{-\infty}^{\infty} \overset{I}{\Phi}_{\underline{k}}^{\times}(\underline{r}',t')\, V(\underline{r}')\, K^{+}(\underline{r}-\underline{r}',t)\, dt\, d^3\underline{r} \quad (401)$$

Using the more general form of the identity (396) [cf. footnote therein] and the relation (369), we arrive at

$$K^{+}(\underline{r}-\underline{r}',t-t') = i\theta(t-t')\langle 0|\left[\psi(\underline{r},t), \psi^{*}(\underline{r}',t')\right]|0\rangle \quad (402)$$

It is customary to call

$$R(\underline{r}-\underline{r}',t-t') \equiv -i\theta(t-t')\left[\psi(\underline{r},t), \psi^{*}(\underline{r}',t')\right] \quad (403)$$

the retarded or causal commutator. (Note that for the case $t=t'$ if there is an interaction between the particles, the commutator is not a c-number but an operator.) In terms of the average value of the retarded commutator between the vacuum states the Green's function is given by

$$K^{+}(\underline{r}-\underline{r}',t-t') = -\langle 0|R(\underline{r}-\underline{r}',t-t')|0\rangle \quad (404)$$

Equation (401) can now be re-cast as follows:

$$M = \overset{I}{\Phi}_{\underline{k}}^{*}(\underline{r},0) - \frac{i}{\hbar}\iint \overset{I}{\Phi}_{\underline{k}}^{*}(\underline{r}',t')\, V(\underline{r}')\langle 0|R(\underline{r}-\underline{r}',t-t')|0\rangle\, dt\, d^3\underline{r}' \quad (405)$$

In particular, if there are no interactions present between the particles then $\langle 0|R(\underline{r}-\underline{r}',t-t')|0\rangle$ can be replaced by $R(\underline{r}-\underline{r}',t-t')$

Now we return to the Lippmann-Schwinger equation. Any one of the equations (398), (401) and (405) can be used as the starting point. However, we employ equation (398). The time integration can be immediately performed by making the time dependence of the integrand more obvious:

$$\langle 0|P\left(\psi(\underline{r}',t)\,\psi^{*}(\underline{r},0)\right)|0\rangle = \theta(t)\langle 0|\psi(\underline{r}',t)\,\psi^{*}(\underline{r},0)|0\rangle \tag{406}$$

This simple relationship can be seen by considering the cases $t>0$ and $t<0$ and the definition of the step-function.

Henceforth we assume that there exists no interaction between the particles, so that $\psi|0\rangle = 0$ always. We adopt a standard trick of the quantum field theory -- that of inserting a complete set of suitably chosen states denoted by the kets $|\alpha\rangle$ No further conditions on the set of states $|\alpha\rangle$ is necessary than that they form a complete set. In the present case they are required to contain all the one-particle bound states in momentum representation. We know that

$$\mathcal{H}|\alpha\rangle = E_\alpha|\alpha\rangle$$

Inserting $\sum_\alpha |\alpha\rangle\langle\alpha| = 1$ in between $\psi(\underline{r}',t)$ and $\psi^{*}(\underline{r},t)$ in equation (406) we get

$$\theta(t)\sum_\alpha \langle 0|\psi(\underline{r}',t)|\alpha\rangle\langle\alpha|\psi^{*}(\underline{r},0)|0\rangle$$

The summation goes only over the one-particle states, because if we have more than one creation operator -- say two -- the uncompensated operator operating on the bra vacuum will always

give zero.

Now we recall that in the Heisenberg representation

$$\psi(\underline{r}',t) = e^{i/\hbar t \mathcal{H}} \psi(\underline{r}',0)\, e^{-i/\hbar t \mathcal{H}}$$

Then

$$\langle o|\psi(\underline{r}',t)|\alpha\rangle = e^{-\frac{i}{\hbar}E_\alpha t}\langle o|\psi(\underline{r}',0)|\alpha\rangle \quad (407)$$

using

$$e^{-\frac{i}{\hbar}t\mathcal{H}}|\alpha\rangle = e^{-\frac{i}{\hbar}tE_\alpha}|\alpha\rangle$$

and

$$\langle o|\, e^{\frac{i}{\hbar}t\mathcal{H}} = \langle o|$$

Resorting to the plane wave representation for $\Phi_{\hat{\underline{k}}}(\underline{r},t)$

$$\Phi^{\times}_{\hat{\underline{k}}}(\underline{r},t) \sim e^{-\frac{i}{\hbar}E_{k'}t}\, e^{i\underline{k}\cdot\underline{r}}$$

We arrive at the following expression for M:

$$M = \Phi^{\times}_{\hat{\underline{k}}}(\underline{r},0) - \frac{i}{\hbar}\iint \sum_\alpha e^{\frac{i}{\hbar}(E_{k'}-E_\alpha)t}\, \theta(t)\, e^{-i\hat{\underline{k}}\cdot\underline{r}}\, V(r')\langle o|\psi(\underline{r}',0)|\alpha\rangle \langle\alpha|\psi^*(\underline{r},0)|o\rangle\, dt\, d^3\underline{r}' \quad (408)$$

The time integration can be performed using the limiting procedure:

$$\lim_{t\to\infty} f(t) = \lim_{\eta\to+0} \eta\int_0^\infty e^{-\eta t'} f(t')\, dt'$$

Replacing $\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(E_{k'}-E_\alpha)t}\,\Theta(t)\,dt = \int_0^{\infty} e^{\frac{i}{\hbar}(E_{k'}-E_\alpha)t}\,dt$

by $\lim_{t\to\infty} \int_0^t e^{\frac{i}{\hbar}(E_{k'}-E_\alpha)t''}\,dt''$

we can prove

$$\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(E_{k'}-E_\alpha)t''}\,\Theta(t'')\,dt'' = \frac{\hbar}{i}\lim_{\eta\to 0}\frac{1}{E_{k'}-E_\alpha+i\eta}$$

Therefore

$$M = \underline{\Phi}_{\underline{k}}(\underline{r},0) + \lim_{\eta\to+0}\int\sum_{\alpha}\frac{\underline{\Phi}^{x}(\underline{r})\,V(\underline{r}')}{E_{k'}-E_\alpha+i\eta}\langle 0|\Psi(\underline{r}',0)|\alpha\rangle \langle\alpha|\Psi^{*}(\underline{r},0)|0\rangle\,d^3\underline{r}' \qquad (409)$$

where we use $\underline{\Phi}(\underline{r},0) \equiv \underline{\Phi}(\underline{r}) \equiv e^{i\underline{k}\cdot\underline{r}}$ for the unperturbed free state.

Now we set $\langle 0|\Psi(\underline{r},0)|\alpha\rangle = \underline{\Psi}_\alpha(\underline{r})$. We can prove that $\underline{\Psi}_\alpha(\underline{r})$ satisfies the one-particle Schrodinger eqn.

$$H\,\underline{\Psi}_\alpha(\underline{r}) = E_\alpha\,\underline{\Psi}_\alpha(\underline{r}) \qquad (409a)$$

where $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r})$

This means that $\Psi_\alpha(\underline{r})$ is a wave function in coordinate representation. It is easily seen that

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\langle 0|\Psi(\underline{r},t)|\alpha\rangle = E_\alpha e^{-\frac{i}{\hbar}E_\alpha t}\langle 0|\Psi(\underline{r},0)|\alpha\rangle$$

Replacing $-\frac{\hbar}{i}\frac{\partial}{\partial t}$ by H,

$$H\langle 0|\Psi(\underline{r},t)|\alpha\rangle = E_\alpha e^{-\frac{i}{\hbar}E_\alpha t}\langle 0|\Psi(\underline{r},0)|\alpha\rangle$$

Since this is true for all values of t, put t = 0. Then we get

$$H\langle 0|\Psi(\underline{r},0)|\alpha\rangle = E_\alpha\langle 0|\Psi(\underline{r},0)|\alpha\rangle$$

which is the same as equation (409a).

Then equation (409) can be thrown in the form

$$M = \underline{\Phi}^{\times}_{\hat{\underline{k}}}(\underline{r},0) + \lim_{\eta\to 0}\sum_\alpha \frac{1}{E_{k'}-E_\alpha+i\eta}\left(\underline{\Phi}_{\hat{\underline{k}}}, V\underline{\Psi}_\alpha\right)\underline{\Psi}^{\times}_{\alpha}(\underline{r}) \qquad (410a)$$

where we employ the notation

$$\left(\underline{\Phi}_{\hat{\underline{k}}}, V\underline{\Psi}_\alpha\right) \equiv \int \underline{\Phi}^{\times}_{\hat{\underline{k}}}(\underline{r}')\, V(\underline{r}')\, \underline{\Psi}_\alpha(\underline{r}')\, d^3\underline{r}'$$

Taking the complex conjugate of equation (410a) and remembering that V is hermitian, we arrive at

$$M^{\times} = \underline{\Psi}^{-}_{\hat{\underline{k}}}(\underline{r}) = \underline{\Phi}_{\hat{\underline{k}}}(\underline{r},0) + \sum_\alpha \frac{1}{E_{k'}-E_\alpha-i\eta}\left(\underline{\Psi}_\alpha, V\underline{\Phi}_{\hat{\underline{k}}}\right)\underline{\Psi}_\alpha(\underline{r})$$

We now write

$$\frac{1}{E_{k'}-E_\alpha-i\eta}\underline{\Psi}_\alpha = \frac{1}{E_{k'}-H-i\eta}\underline{\Psi}_\alpha$$

since Ψ_α is an eigenstate of H with eigenvalue E_α .

Therefore

$$\Psi^-_{\hat{k}}(\underline{r}) = \Phi_{\hat{k}}(\underline{r},0) + \sum_\alpha \frac{1}{E_{k'} - H - i\eta} \left(\Psi_\alpha, V\Phi_{\hat{k}}\right) \Psi_\alpha(\underline{r})$$

Because of the completness of Ψ_α we can substitute

$$\sum_\alpha \left(\Psi_\alpha, V\Phi_{\hat{k}}\right) \Psi_\alpha(\underline{r}) = V\Phi_{\hat{k}} \quad \text{in the above equation;}$$

$$\Psi^-_{\hat{k}}(\underline{r}) = \Phi_{\hat{k}}(\underline{r},0) + \frac{1}{E_{k'} - H - i\eta} V\Phi_{\hat{k}}(\underline{r}) \qquad (410b)$$

This is just the Lippmann-Schwinger equation in the coordinate representation. Thus we have proved that the matrix element $\langle 0|\Psi(\underline{r},0)|\Psi^-_{\hat{k}}\rangle$ is a wave function in the configuration space corresponding to outgoing wave. So the assumption with which we have started the computation is correct. The choice

$$S_{\hat{k}\hat{k}_0} = \left(\Psi^-_{\hat{k}}, \Psi^+_{\hat{k}_0}\right)$$

is therefore valid, because, the T matrix to which it leads, yields the one-particle wave function.

In the course of our computations we have encountered a number of interesting results. The alternative forms of M enable us to study the analytic properties of the S-matrix in terms of the retarded commutator. The two major tricks employed to arrive at the desired result are:

(i) Expressing the time-ordered product in terms of retarded commutator.

(ii) Insertion of a complete set $\sum_\alpha |\alpha\rangle\langle\alpha| = 1$

in between $\Psi(\underline{r}',t)$ and $\Psi^*(\underline{r},0)$ to bring out the time dependence explicitly.

and (iii) Replacement of true fields by "in" or "out" fields. This is unavoidable in the case of interactions which introduces non-local potentials.

We wish to consider briefly the following points.

(i) Causality in the framework of field theoretic approach

and (ii) The emergence of the spectral representation for ρ_γ used in Chapter III [cf. equation (53)] from field equations and the retarded commutator.

Consider the following expression for M [equation (405)]

$$M = \Phi^{\times}_{\underline{k}}(\underline{r}) = \frac{i}{\hbar}\iint \Phi^{\times}_{\underline{k}}(\underline{r}',t)\, V(\underline{r}')\langle 0|R(\underline{r}-\underline{r}',t)|0\rangle\, dt\, d^3\underline{r}$$

where $R(\underline{r}-\underline{r}',t) = -i\theta(t)\left[\Psi(\underline{r},t), \Psi^*(\underline{r}',0)\right]$

Clearly the integral in equation (405) is a Fourier transform, because $\Phi^{\times}_{\underline{k}}$ is essentially a plane wave $e^{-i\underline{k}.\underline{r}}$.

So the expression for M contains the Foruer transform of a causal function R. If the potential obeys certain restrictions then M is analytic in the upper half of the complex k-plane. So, the causal property appears natually in field theoretic approach and it is only this which makes the T matrix (and hence the scattering amplitude, for T and f are related as will be shown later) analytic in the upper half plane. Therefore a dispersion relation is possible for the scattering amplitude. However, we must know more about the behaviour of the

potential. The behaviour for large k must be known. Therefore we cannot go too far in the case of potential scattering.

On the other hand in relativistic quantum field theory there is no concept of potentials and the analytid properties follow from the properties of the retarded commutator.

Again consider the matrix element M in the Form:

$$M = \Phi^{x}_{\underline{k}}(\underline{r}) + \lim_{\eta \to 0} \sum \frac{1}{E_{k'} - E_{\alpha} + i\eta} \int \Phi^{x}_{\underline{k}}(\underline{r}) V(\underline{r}') \psi_{\alpha}(\underline{r}') \psi^{x}_{\alpha}(\underline{r}) \, d^3\underline{r}' \qquad (411)$$

The summation over α includes bound states as well as continuum states. This is made explicit by writing

$$\sum_{\alpha} \frac{1}{E_{k'} - E_{\alpha} + i\eta} \psi_{\alpha}(\underline{r}') \psi^{x}_{\alpha}(\underline{r}) = -\frac{2m}{\hbar^2} \sum_{\substack{\text{Bound} \\ \text{States}}} \frac{\psi_B(\underline{r}') \psi^{x}_B(\underline{r})}{k^2 - k_B^2} + \frac{2m}{\hbar^2} \int \frac{\psi_{k''}(\underline{r}') \psi^{x}_{k''}(\underline{r})}{k^2 - k''^2 + i\eta} dk''$$

$$\left[E_{k'} = \frac{\hbar^2 k'^2}{2m} \right] \qquad (412)$$

But the right hand side of equation (412) is precisely what we denoted by $2m/\hbar^2 \, g_{\gamma}(\underline{r}, \underline{r}'; k)$

In our previous discussion (Chapter III equation (53)) we quoted a mathematical theorem to support the contention that the spectral decomposition of g_{γ} is possible. However in the present case we did not resort to analytic properties of g_{γ}. The

decomposition arises automatically from the field equations and the retorded commutator,

Replacing $\sum_{\alpha} \frac{1}{E_{k'} - E_{\alpha} + i\eta} \Psi_{\alpha}(\underline{r}') \Psi_{\alpha}(\underline{r})$ in equation (411) by $2m/\hbar^2 \, \varrho_{\gamma}$,

$$M = \Phi^{\times}_{\hat{\underline{k}}} + \frac{2m}{\hbar^2} \int \Phi^{\times}_{\hat{\underline{k}}} V \varrho_{\gamma} \, d^3\underline{r} \qquad (413)$$

Substituting equation (413) in the expression for

$$T_{\hat{\underline{k}}\underline{k}_0} = \int M(\underline{r}) V(\underline{r}) \Phi_{\underline{k}_0}(\underline{r}) \, d^3\underline{r} \, ,$$

we get

$$\frac{2m}{\hbar^2} T_{\hat{\underline{k}}\underline{k}_0} = \int e^{-i(\hat{\underline{k}} - \underline{k}_0).\underline{r}} U(\underline{r}) \, d^3\underline{r} + \iint e^{-i\hat{\underline{k}}.\underline{r}'} e^{i\underline{k}_0.\underline{r}} U(\underline{r}) \varrho_{\gamma}(\underline{r}, \underline{r}'; k) U(\underline{r}') \, d^3\underline{r} \, d^3\underline{r}'$$

It is seen easily that the first term of the above equation is the first Born approximation. So we immediately write down the relation between the scattering amplitude and T matrix

$$f(k, \Delta) = -\frac{2m}{\hbar^2} T_{\hat{\underline{k}}\underline{k}_0}$$

where $\Delta = \hat{\underline{k}} - \underline{k}_0$

R É S U M É:

To summarise this discussion, let us recall that at the very beginning we possessed little knowledge of scattering processes. We assumed the Schrödinger equation and solved it for continuous eigenvalues. We defined a Green's function,

and hence derived the scattering amplitude. This led to dispersion relations in terms of the momentum and momentum transfer, and later in terms of energy. There was a maximum limit imposed on the energy, and while removing this we derived the Mandelstam representation. This is feasible in potential scattering but not in general.

In order to study the analytic properties of the scattering amplitude with respect to the momentum transfer, we had to find its asymptotic behaviour for large t. This was facilitated by Regge's theory. Making use of the Sommerfeld-Waston theorem, we expressed the scattering amplitude to terms of a continuous variable ℓ. We found that the asymptotic behaviour depended upon the bound state or resonance corresponding to the largest angular momentum. Hence we determined the maximum number of substractions to be made. Thus, although the Regge theory did not enable us to find directly all the possible bound states and resonances, it did allow us to write down a dispersion relation. The Mandelstam representation thus obtained was valid everywhere in the topological product of the cut s and t planes, and for a wide but restricted class of potentials.

The above theory would have compelled us to determine the discontinuity function ρ by the "strip approximation" method. The avoid complications, we projected the partial wave amplitudes. The equations for these consisted of only one integral equation and some quadratures, or, in the more general case, of a limited number of uncoupled integral equations.

The simplicity of these non-linear equations suggested the N/D method of solution, and the equations were reduced to non-singular Fredholm integral equations.

Such a method of solution was completely justified later by the properties of the Jost functions. These were introduced by first attacking the problem in the more abstract formalism of the S-matrix. We defined in and out states and derived the Lippmann-Schwinger equation. We obtained also the T operator whose analogue was the scattering amplitude function. The angular momentum representation was found to be a convenient one for the S operator, and as a by-product we bbtained the Jost functions. These functions were found to be of great use, especially in the analytic extension of the S-matrix to the complex plane, where its poles could be easily interpreted in physical terms.

We described also the time-dependent approach by using the causality principle. By confining the scattering processes to a "black box" and imposing restrictions of a causal nature on the output, we obtained some relations between input and output. These were, however, too general because of the necessarily weak restriction imposed by causality.

Towards the end, we abandoned the one-particle point quantum mechanics and turned to quantum field theory. Here we defined in and out operators and a vacuum states. Using these and the commutators for the field operators, we were able to establish all the old relations but in a much more natural way.