



Archivo
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I. Group Theoretical Preliminaries.

1.1 If u ^{does} not contain explicitly the time, the necessary and sufficient condition to be a constant of motion is:

$$[u, H] = 0$$

Infin. contact transf:

$$q_i \rightarrow q'_i = q_i + \delta q_i$$

$$p_i \rightarrow p'_i = p_i + \delta p_i$$

The generating functin F of this transf. is:

$$F = \sum_i q_i p'_i + \epsilon G(q, p')$$

ϵ is the infinitesimal parameter and is customary call G the generating functin.

It may be shown that:

$$\delta u = \epsilon [u, G]$$

In particular:

$$\delta H = \epsilon [H, G]$$

All the constants of motion are the generating functions of those infinitesimal contact transformations which leave the Hamiltonian invariant.

If the angular moment is a constant of motion, the group of the Hamiltonian contains the group $SO(3)$.

1.2 A group is defined as a set of elements among which a law of composition is established, such that the composition of any two elements a and b of the group, taken in this order, is an element of the set and satisfy the following conditions:

1. The associative law $c(ba) = (cb)a$

2. There exists a unit element 1 , which leaves any element a unaltered on composition with it.

$$1a = a1 = a$$

3. To each element a corresponds an inverse a^{-1} which gives, on composition with a , the unit element:

$$aa^{-1} = a^{-1}a = 1$$

The number of elements in a group, its order, may be finite or not.

A subgroup h of a group g is a set of elements of g which itself fulfills the group conditions.

The set of all nonsingular linear homogeneous transf. on an n -dimensional vector space (we suppose the transf. matrices to have complex coeff.) form the full linear group $GL(n)$. Restriction of these transf. to unitary transf. give us the unitary group $U(n)$ and:

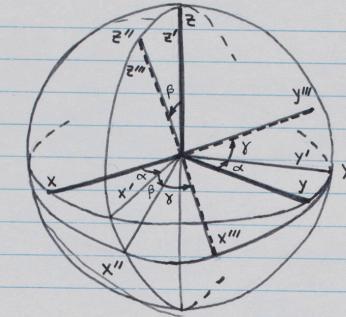
$$U(n) \subset GL(n)$$

If we take the further restriction that the unitary matrices have $\det +1$, i.e. are unimodular, result the special unitary group $SU(n)$. The group of all real linear homogeneous transf. on an n -dimensional space which preserve the distance between two points (in Euclidean sense) i.e. the rotations and reflections about the origin is called the orthogonal group $O(n)$. We shall be concerned particularly with the three-dimensional unimodular orthogonal group $SO(3)$.

To specify any element of $GL(n)$ we would need n^2 complex numbers. In the case of the rotation group $O(3)$ we need only three real numbers, corresponding to the well-known fact that any rotation is completely specified by three real numbers.

1.3 Euler angles:

We shall assume a right-handed frame of axes. We perform three successively positive rotations in the order:



1. A rotation α ($0 \leq \alpha \leq 2\pi$) about the z axis ($S \rightarrow S'$)
(This axis is commonly called vertical)

2. A rotation β ($0 \leq \beta \leq \pi$) about the y' axis (called the line of nodes) ($S' \rightarrow S''$)

3. A rotation γ ($0 \leq \gamma \leq 2\pi$) about the z'' axis (called figure axis) ($S'' \rightarrow S'''$)

It should be noted that the polar coordinates ϕ, θ with respect to the original frame S of the z -axis ~~are~~ in its final position S''' are identical with the Euler angles α, β, γ respectively.

1.4 We mean by a representation of degree n of a group G that to every element a of G is assigned a linear transf. $T(a)$ on a vector space P_n of dimension n in such a way that these linear transf. obey the law of composition

$$T(a) \cdot T(b) = T(ab)$$

If to each group element corresponds a distinct transf., we call it a faithful representation.

When a definite coordinate system is chosen in the space P_n each transf. $T(a)$ corresponds to a square nonsingular matrix. The orthogonal unit vectors which establish this coordinate system are called the basis of the representation.

If we replace the coordinate system by another obtained from it by a transf. S , the group element a will be represented by the transf. $S T(a) S^{-1}$. We have again a representation of G , which is said to be equivalent to the former one.

Suppose there exists a subspace R' of R such that all vectors lying in this subspace are transformed by a given transf. T into vectors of R' . We say that the subspace R' is invariant under the transf. T . If R' is invariant under all transf. $T(a)$ representing the group G , the transf. $T'(a)$ which are induced in R' themselves give a representation of G . If we picture the transf. as matrices, then we may choose such a basis that all the representation matrices in a given representation take the form:

P	R
R	Q

where the submatrix P corresponds to the transf. on the subspace R' . (The rectangular submatrix R will usually, but not necessarily, contain nothing but zeros). A representation based on a space R is called irreducible if R contains no subspace other than itself and the null space which is invariant under the transf. $T(a)$ representing the group G .

Spinors.

We will consider a system with angular momentum $S = \frac{1}{2}$. The components of the angular momentum operator S , shortly the spin, are: (Cf. Edmonds p. 17)

$$S_x = \frac{i}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_y = \frac{i}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_z = \frac{i}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Since $2S+1$ in this case is 2, there are only two basis "vectors", called spinors and written ψ_+ and ψ_- . An arbitrary spinor can be written as:

$$\underline{\psi} = c_+ \underline{\psi}_+ + c_- \underline{\psi}_-$$

where c_+ and c_- are the spinor components. It is usual to write this as a 1 column, 2 row matrix:

$$\underline{\psi} = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

The coefficients c 's must be complex; otherwise we would have only two numbers to describe a rotation, and this is not enough. It may appear that having four numbers is more than necessary. After all, a vector needs only three numbers to describe it. Actually this is due to the fact that a vector has no "thickness"; if we should rotate a vector around its own axis, we would be unable to detect any effect on it. A spinor, on the other hand, is sensible to such a rotation.

The inner product in spinor space is defined as follows:

If: $\underline{\psi} = c_+ \underline{\psi}_+ + c_- \underline{\psi}_-$, $\underline{\varphi} = d_+ \underline{\psi}_+ + d_- \underline{\psi}_-$ then:

$$(\underline{\psi}, \underline{\varphi}) = c_+^* d_+ + c_-^* d_-$$

and the square of magnitude:

$$|\underline{\psi}|^2 \equiv (\underline{\psi}, \underline{\psi}) = |c_+|^2 + |c_-|^2$$

Let us investigate the transformation properties of a spinor. For this we need to know some of the mathematical properties of S . If we write

$$\underline{S} = \frac{\hbar}{2} \underline{\sigma}$$

Then we get for the components of \underline{S} the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

with the properties:

$$\sigma_i^2 = 1$$

$$i = x, y, z$$

$$\left. \begin{array}{l} \sigma_i \sigma_k - \sigma_k \sigma_i = 2i \delta_{ik} \\ \sigma_i \sigma_k + \sigma_k \sigma_i = 2\delta_{ik} \end{array} \right\} \quad i, k, l \text{ any cyclic permutation of } x, y, z.$$

and: $\sigma_i^n = \begin{cases} \sigma_i & \text{for } n \text{ odd} \\ 1 & \text{for } n \text{ even.} \end{cases}$

If we rotate the spinor $\underline{\psi} = c_+ \underline{u}_+ + c_- \underline{u}_-$ through an angle θ around an axis \underline{n} , we obtain a new spinor $\underline{\psi}'$:

$$\underline{\psi}' = R_\theta(\underline{n}) \underline{\psi}$$

$\underline{\psi}'$ can be written either as $\underline{\psi}' = c'_+ \underline{u}_+ + c'_- \underline{u}_-$ or
 $\underline{\psi}' = c_+ \underline{u}'_+ + c_- \underline{u}'_-$

We ask for the form of the operator $R_\theta(\underline{n})$ when the latter form is obtained, i.e. the components of $\underline{\psi}'$ remain the same, and we ask for the transformation properties of the "spinor basis".

Let the amount of rotation be infinitesimal and the axis of rotation be the z -axis. Then:

$$R_{dz}(\underline{z}) = 1 + r_z d\theta = 1 - \frac{i}{\hbar} S_z d\theta = 1 - \frac{i}{2} \sigma_z d\theta$$

If we repeat this process n times, then the spinor will be rotated through a finite angle $\theta = n d\theta$ and:

$$R_\theta(\underline{z}) = (R_{dz}(\underline{z}))^n = (1 - \frac{i}{2} \sigma_z d\theta)^n$$

Since $d\theta$ is an infinitesimal, we can make use of the relation:

$$(1 + S)^n = e^{nS} \quad (\text{for small } S)$$

Hence: $R_\theta(\underline{z}) = e^{-\frac{i}{2} \sigma_z n d\theta} = e^{-\frac{i}{2} \sigma_z \theta}$

If we now make use of the expansion:

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots$$

we get:

$$R_\theta(\underline{z}) = 1 - i \sigma_z \frac{\theta}{2} - \frac{(\frac{\theta}{2})^2}{2!} + i \sigma_z \frac{(\frac{\theta}{2})^3}{3!} + \frac{(\frac{\theta}{2})^4}{4!} - \dots$$

$$= \cos \frac{\theta}{2} - i \sin \frac{\theta}{2} \cdot \sigma_z = \begin{pmatrix} \cos \frac{\theta}{2} - i \sin \frac{\theta}{2} & 0 \\ 0 & \cos \frac{\theta}{2} + i \sin \frac{\theta}{2} \end{pmatrix}$$

$$\therefore R_\theta(\underline{z}) = \begin{pmatrix} e^{-\frac{i\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix}$$

Similarly:

$$R_\theta(\underline{x}) = \cos \frac{\theta}{2} - i \sin \frac{\theta}{2} \cdot \sigma_x = \begin{pmatrix} \cos \frac{\theta}{2} & -i \sin \frac{\theta}{2} \\ -i \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix}$$

$$R_\theta(\underline{y}) = \cos \frac{\theta}{2} - i \sin \frac{\theta}{2} \cdot \sigma_y = \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix}$$

If we want the matrix for a rotation around an arbitrary axis, we can use the Euler angles (Cf. Goldstein p. 107 and 116, but we use here the convention of the preceding section). Hence:

$$R = \begin{pmatrix} e^{-i\frac{\psi}{2}} & 0 \\ 0 & e^{i\frac{\psi}{2}} \end{pmatrix} \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix} \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{i\frac{\phi}{2}} \end{pmatrix}$$

Let us consider a few simple examples:

1. Rotate $\underline{\psi} = c \underline{u}_+ = \begin{pmatrix} c \\ 0 \end{pmatrix}$ through an angle π around the x axis:

$$\underline{\psi}' = R_\pi(\underline{x}) \underline{\psi} = \begin{pmatrix} \cos \frac{\pi}{2} - i \sin \frac{\pi}{2} & 0 \\ -i \sin \frac{\pi}{2} & \cos \frac{\pi}{2} \end{pmatrix} \begin{pmatrix} c \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -ic \end{pmatrix} = -ic \underline{u}_-$$

2. Rotate $\underline{\psi} = c \underline{u}_+ = \begin{pmatrix} c \\ 0 \end{pmatrix}$ through an angle π around the y axis:

$$\underline{\psi}'' = R_\pi(\underline{y}) \underline{\psi} = \begin{pmatrix} \cos \frac{\pi}{2} & -\sin \frac{\pi}{2} \\ \sin \frac{\pi}{2} & \cos \frac{\pi}{2} \end{pmatrix} \begin{pmatrix} c \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ c \end{pmatrix} = c \underline{u}_+$$

Thus we obtain the surprising result that a rotation through π around x of a spinor pointing in the z direction differs from a rotation through π around y . For a vector we would expect in both cases the result to be $c \underline{u}_-$. This just indicates what we have mentioned

before, namely that a vector has no thickness. The two rotations performed above differ by a rotation through π around z :

$$R_{\pi}(z) \underline{\psi}' = \begin{pmatrix} e^{-i\frac{\pi}{2}} & 0 \\ 0 & e^{i\frac{\pi}{2}} \end{pmatrix} \begin{pmatrix} 0 \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ -ic \end{pmatrix} = \underline{\psi}''$$

$$R_{\pi}(z) \underline{\psi}'' = \begin{pmatrix} e^{i\frac{\pi}{2}} & 0 \\ 0 & e^{-i\frac{\pi}{2}} \end{pmatrix} \begin{pmatrix} 0 \\ -ic \end{pmatrix} = \begin{pmatrix} 0 \\ ic \end{pmatrix} = \underline{\psi}'$$

3. Rotate $\underline{\psi}$ around the z -axis by angle θ :

$$\underline{\psi}' = R_{\theta}(z) \underline{\psi} = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix} \begin{pmatrix} c \\ 0 \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\theta}{2}}c \\ 0 \end{pmatrix} = e^{-i\frac{\theta}{2}}c \underline{u}_+$$

4. Rotate $\underline{\psi}$ around the y -axis by $\frac{\pi}{2}$:

$$\underline{\psi}' = R_{\frac{\pi}{2}}(y) \underline{\psi}' = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} c \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{c}{\sqrt{2}} \\ \frac{c}{\sqrt{2}} \end{pmatrix} = \frac{c}{\sqrt{2}} (\underline{u}_+ + \underline{u}_-)$$

5. Rotate around any axis by 2π . Then we find that:

$$\underline{\psi}' = -\underline{\psi}$$

This example shows that spinors are a two-valued representation. Does this violate any law of nature? No. The only quantities that can be measured or observed physically are bilinear expressions of the form $(\underline{\psi}, \underline{\psi})$ and these are always single-valued, even for spinors.

We can use our basis spinors, in the way we used basis vectors, to construct systems characterized by angular momentum made up out of sums or differences of $S = \frac{1}{2}$. Thus we can form the direct product of the basis spinors:

$$\underline{u}_+ \underline{u}_+ \rightarrow V+$$

$$\frac{1}{\sqrt{2}} (\underline{u}_+ \underline{u}_- + \underline{u}_- \underline{u}_+) \rightarrow V_0$$

$$\underline{u}_- \underline{u}_- \rightarrow V-$$

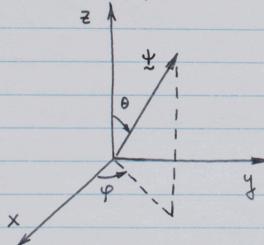
The three V 's are the three components of a system of total angular momentum $= \frac{1}{2} + \frac{1}{2} = 1$, hence this is a system that has transformation properties of a vector. One could say that a

vector in ordinary space is a tensor of second rank in spinor space.

If instead of taking the three possible symmetric direct products we would take the only possible asymmetric one $\underline{u}_+ \underline{u}_- - \underline{u}_- \underline{u}_+$, we obtain a system with just one element necessary to describe it and total angular momentum 0, i.e. obviously a scalar. All the above direct products are bilinear in the spinors and hence single-valued, as vectors and scalars ought to be.

We have said above that a certain spinor was pointing in the z direction. That statement must now be explained. As was pointed out before, a spinor is described by four quantities and since what we ordinarily mean by direction needs only three numbers to be completely specified, we shall ascribe to a spinor a direction and a phase.

By the direction of a spinor $\underline{\psi} = c \underline{u}_+ + c_- \underline{u}_-$ we mean the direction of the z axis of a coordinate system in which the spinor is expressed by $\underline{\psi}' = c \underline{u}_+$. As is suggested by the diagram,



we must rotate the spinor through an angle φ around the z -axis and through an angle θ around the y -axis in order to have $\underline{\psi}' = c \underline{u}_+$. The angle φ is the phase angle and the spinor is considered to be lined up with the z -axis only when both θ and φ are reduced to zero. Thus in order to know the direction and phase of a spinor, we must find θ and φ . These we can find from c_+ and c_- as follows: Consider the spinor to be lined up with the z -axis so that

$$\underline{\psi}' = c \underline{u}_+ = \begin{pmatrix} c_+ \\ 0 \end{pmatrix}$$

We can bring it into the position where $\underline{\psi} = c \underline{u}_+ + c_- \underline{u}_- = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$ by reversing the order of rotations:

$$\hat{\psi}'' = R_\theta(\hat{y}) \hat{\psi}' = \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix} \begin{pmatrix} c \\ 0 \end{pmatrix} = \begin{pmatrix} c \cos \frac{\theta}{2} \\ c \sin \frac{\theta}{2} \end{pmatrix}$$

$$\hat{\psi} = R_\varphi(\hat{z}) \hat{\psi}'' = \begin{pmatrix} e^{-i\frac{\varphi}{2}} & 0 \\ 0 & e^{i\frac{\varphi}{2}} \end{pmatrix} \begin{pmatrix} c \cos \frac{\theta}{2} \\ c \sin \frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} ce^{-i\frac{\varphi}{2}} \cos \frac{\theta}{2} \\ ce^{i\frac{\varphi}{2}} \sin \frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} c+ \\ c- \end{pmatrix}$$

Hence:

$$\cot \frac{\theta}{2} = \frac{|c+|}{|c-|}$$

and $\varphi = (\text{phase of } c-) - (\text{phase of } c+)$

By a spinor field we mean a field at every point of which a spinor is prescribed:

$$\hat{\Psi}(x, y, z) = \hat{\psi}_+(x, y, z) \hat{u}_+ + \hat{\psi}_-(x, y, z) \hat{u}_-$$

The angular momentum operator for spinor fields consists of two parts (analogously to the vector field case):

$$\hat{J} = \hat{L} + \hat{S}$$

and the eigenfunctions are:

$$\begin{aligned} \hat{\Psi}_{J, L, M} = C_{L, \frac{1}{2}}(J, M; M - \frac{1}{2}, \frac{1}{2}) Y_{L, M - \frac{1}{2}} \hat{u}_+ + \\ + C_{L, \frac{1}{2}}(J, M; M + \frac{1}{2}, \frac{1}{2}) Y_{L, M + \frac{1}{2}} \hat{u}_- \end{aligned}$$

where J can be only $L + \frac{1}{2}$ or $L - \frac{1}{2}$. If $J = L + \frac{1}{2}$ we have the stretched case:

$$\hat{\Psi}_{J, L, M=J} \sim Y_{LL} \hat{u}_+$$

$$\hat{\Psi}_{J, L, M=J-1} = J_- \hat{\Psi}_{J, L, M=J}$$

If $J = L - \frac{1}{2}$:

$$\hat{\Psi}_{J, L, J} = a Y_{L, L-1} \hat{u}_+ + b Y_{L, L} \hat{u}_-$$

$$\hat{\Psi}_{J, L, J-1} = J_- \hat{\Psi}_{J, L, J}$$

where the coefficients a, b are found from $J_+ \hat{\Psi}_{J, L, J} = 0$

Dirac Equation

There is experimental evidence (e.g. the Stern-Gerlach experiment) that the intrinsic angular momentum of the electron is half-integer. Therefore, we assume, after Pauli, that the electron wave function is a spinor field and we would like to obtain the equation for this field. We will approach this problem by trying to build a formalism for spinor fields in as close analogy as possible to the formalism for the vector fields E and H of the electromagnetic field.

We therefore, in the first place, assume the existence of two, and not one, spinors $\hat{\Psi}$ and $\hat{\Psi}^\dagger$ in analogy to the two vectors E and H . This shouldn't be very surprising, since for any field, with the exception of scalar fields, some such extension is necessary to have the equations of the field invariant under the Lorentz transformation. (For example, one way of making the equations of motion in classical mechanics relativistically invariant is to treat time as a fourth coordinate.)

Next, we want the wave equation satisfied by the electron. We want this to be relativistically correct. We know that the relation between mass, momentum and energy of a particle in free space is

$$p^2 c^2 + m^2 c^4 = E^2$$

If we recall that the operators for momentum and energy are:

$$p \rightarrow \frac{t}{i} \nabla \quad E \rightarrow i \hbar \frac{\partial}{\partial t}$$

the preceding equation in operator form becomes:

$$-c^2 t^2 \nabla^2 + m^2 c^4 \hat{\Psi}^\dagger = -\hbar^2 \frac{\partial^2 \hat{\Psi}^\dagger}{\partial t^2}$$

or:

$$\nabla^2 \hat{\Psi} - k^2 \hat{\Psi} = \frac{1}{c^2} \frac{\partial^2 \hat{\Psi}}{\partial t^2} \quad (1)$$

where $k = \frac{mc}{\hbar} = \text{reciprocal Compton wavelength}$.

This is the Klein-Gordon equation. However, just as in the case of the electromagnetic field, the wave equation tells us nothing about the relation between the two spinors. We know that each of the

two spinors, or better yet, each of the two components of the two spinors, must satisfy Klein-Gordon's equation. To find out the relation between them, we need the equivalent of Maxwell's which give the relation between E and H . As we know Maxwell's equations in free space are:

$$\begin{aligned} \text{rot } \underline{E} &= -\frac{1}{c} \frac{\partial \underline{H}}{\partial t} & \text{div } \underline{E} &= 0 \\ \text{rot } \underline{H} &= \frac{1}{c} \frac{\partial \underline{E}}{\partial t} & \text{div } \underline{H} &= 0 \end{aligned} \quad \left. \right\} \quad (2)$$

From these relations we obtain the wave equation for the electromagnetic field, making use of the identity:

$$\text{rot rot } \underline{F} = -\nabla^2 \underline{F} + \text{grad div } \underline{F} = -\nabla^2 \underline{F} \quad \text{since } \text{div } \underline{F} = 0$$

We see that the fundamental characteristics of Maxwell's equations are: they are all linear, first order differential equations, and, when iterated, they result in the wave equation. In addition, the operators involved when operating on a vector produce a vector.

Let us therefore introduce an operator which we will call "spin rot", and write $\tilde{\text{rot}}$, such that when it operates on a spinor it produces another spinor. In addition, we want this $\tilde{\text{rot}}$ to be a first order differential operator. The following expression has the required properties:

$$\tilde{\text{rot}} \equiv \underline{\Gamma} \cdot \nabla = \begin{pmatrix} \frac{\partial}{\partial z} & \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} & -\frac{\partial}{\partial z} \end{pmatrix}$$

This is obviously a first order differential operator and to convince ourselves that when operating on a spinor it produces a spinor, we merely note that $\underline{\Gamma}$ transforms as a vector and ∇ transforms also as a vector, hence $(\underline{\Gamma} \cdot \nabla) \underline{\psi}$ must transform as a spinor, and we can prove the relation:

$$\tilde{\text{rot}} \tilde{\text{rot}} \underline{\psi} = \nabla^2 \quad (3)$$

by putting:

$$\tilde{\text{rot}} \tilde{\text{rot}} \underline{\psi} = \sum_{i,k} (\Gamma_i \nabla_i)(\Gamma_k \nabla_k) = \sum_i \Gamma_i^2 \nabla_i^2 + \sum_{i \neq k} (\Gamma_i \Gamma_k + \Gamma_k \Gamma_i) \nabla_i \nabla_k$$

Since $\Gamma_i^2 = 1$ and $\Gamma_i \Gamma_k + \Gamma_k \Gamma_i = 0$ ($i \neq k$) equation (3) follows as an identity. This is similar to the identity that holds for vectors except for the sign of ∇^2 . Furthermore, (3) is somewhat more general since it holds for all spinors, while the corresponding vector identity is restricted to vectors \underline{F} such that $\text{div } \underline{F} = 0$.

We are now ready to write Dirac's equations in analogy to (2) as follows.

$$\begin{aligned} \tilde{\text{rot}} \underline{\psi} &= a_1 \underline{\psi} + a_2 \dot{\underline{\psi}} \\ \tilde{\text{rot}} \dot{\underline{\psi}} &= b_1 \underline{\psi} + b_2 \dot{\underline{\psi}} \end{aligned} \quad \left. \right\} \quad (4)$$

and then by taking either of the two, applying to it the $\tilde{\text{rot}}$ operator and making use of the other equation to obtain an equation containing just one of the spinors, we find that in order that the equation so obtained be identical with the Klein-Gordon equation, we must set:

$$\begin{aligned} a_1 &= i \kappa & a_2 &= \frac{1}{c} \\ b_1 &= -i \kappa & b_2 &= \frac{1}{c} \end{aligned}$$

This choice of the a 's and b 's is not unique unless we require that $a_2 = b_2$. The requirement $a_2 = b_2$ involves no loss of generality (we have four coefficients to find and only three conditions on them), hence we can impose the fourth condition in any arbitrary way, provided it gives us unique solutions for the a 's and b 's.

Hence we finally obtain the Dirac equations in what we call Maxwell form:

$$\begin{aligned} \tilde{\text{rot}} \underline{\psi} - i \kappa \underline{\psi} &= -\frac{1}{c} \dot{\underline{\psi}} \\ \tilde{\text{rot}} \dot{\underline{\psi}} + i \kappa \underline{\psi} &= -\frac{1}{c} \dot{\underline{\psi}} \end{aligned} \quad \left. \right\} \quad (5)$$

Since $\underline{\psi}$ has two components, ψ_+ and ψ_- , and $\dot{\underline{\psi}}$ has also two components, $\dot{\psi}_+$ and $\dot{\psi}_-$, we can talk about a four spinor $\underline{\Psi}$ which has four components:

$$\underline{\Psi} = \begin{pmatrix} \psi_+ \\ \psi_- \\ \varphi_+ \\ \varphi_- \end{pmatrix}$$

and for this $\underline{\Psi}$, called Dirac spinor, we can write the two Dirac equations obtained previously as just one equation. To do this we note that since $\nabla = \frac{i}{\hbar c} \underline{p}$, we can write $\text{rot} = \frac{i}{\hbar c} \underline{\nabla} \cdot \underline{p}$. Also $\underline{E} = i\hbar \frac{\partial}{\partial t}$. Therefore equations (5) become

$$\left. \begin{aligned} \frac{1}{\hbar c} (\underline{\nabla} \cdot \underline{p}) \underline{\Psi} + \kappa \underline{\Psi} &= \frac{\underline{E}}{\hbar c} \underline{\Psi} \\ \frac{1}{\hbar c} (\underline{\nabla} \cdot \underline{p}) \underline{\Psi} - \kappa \underline{\Psi} &= \frac{\underline{E}}{\hbar c} \underline{\Psi} \end{aligned} \right\} \quad (6)$$

These four simultaneous equations can therefore be written as one equation for the Dirac spinor as:

$$\frac{1}{\hbar c} (\underline{\alpha} \cdot \underline{p}) \underline{\Psi} + \beta \kappa \underline{\Psi} \rightarrow \frac{\underline{E}}{\hbar c} \underline{\Psi} \quad (7)$$

where β is the matrix:

$$\beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

and $\underline{\alpha}$ has as its components the matrices:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad (4 \times 4 \text{ matrix})$$

i.e.:

$$\alpha_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad \alpha_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \quad \alpha_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

By direct calculation we check that the α 's anticommute with each other and with β , and in addition:

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1$$

The equation (7) is the Dirac equation for the electron in Dirac form. It is the same equation that we have written before as Dirac equations in "Maxwell form".

Maxwell's Equations in Dirac's Formalism.

In order to get better acquainted with Dirac's formalism, we now write Maxwell's equations for the electromagnetic field in Dirac's form. The two Maxwell equations

$$\text{rot } \underline{H} = \frac{1}{c} \frac{\partial \underline{E}}{\partial t}$$

$$-\text{rot } \underline{E} = \frac{1}{c} \frac{\partial \underline{H}}{\partial t}$$

actually stand for six simultaneous equations for each of the three components of the vectors \underline{E} and \underline{H} . We therefore introduce a six-vector \underline{F} (just like we had to introduce the four spinor $\underline{\Psi}$) with components consisting in the three components of \underline{E} and the three components of \underline{H} :

$$\underline{F} = \begin{pmatrix} \underline{E} \\ \underline{H} \end{pmatrix}$$

Then all the six equations for the components of \underline{F} can be written as a single equation:

$$(\underline{\alpha} \cdot \nabla) \underline{F} = \frac{1}{c} \dot{\underline{F}}$$

To see what $\underline{\alpha} \cdot \nabla$ is in the above equation, we write out the six Maxwell equations:

$$\begin{aligned} -\frac{\partial}{\partial z} H_y + \frac{\partial}{\partial y} H_z &= \frac{1}{c} \dot{E}_x \\ \frac{\partial}{\partial z} H_x - \frac{\partial}{\partial x} H_z &= \frac{1}{c} \dot{E}_y \\ -\frac{\partial}{\partial y} H_x + \frac{\partial}{\partial x} H_y &= \frac{1}{c} \dot{E}_z \\ \frac{\partial}{\partial z} E_y - \frac{\partial}{\partial y} E_z &= \frac{1}{c} \dot{H}_x \\ -\frac{\partial}{\partial x} E_y + \frac{\partial}{\partial y} E_x &= \frac{1}{c} \dot{H}_y \\ \frac{\partial}{\partial x} E_z - \frac{\partial}{\partial z} E_x &= \frac{1}{c} \dot{H}_z \end{aligned}$$

$E_x \quad E_y \quad E_z \quad H_x \quad H_y \quad H_z$

Now since $\underline{\alpha} \cdot \nabla = \alpha_x \frac{\partial}{\partial x} + \alpha_y \frac{\partial}{\partial y} + \alpha_z \frac{\partial}{\partial z}$, we see immediately that α 's the α 's must be

$$\alpha_x^F = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\alpha_y^F = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\alpha_z^F = \begin{pmatrix} 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Instead of above, we can write

$$\alpha_x^F = \begin{pmatrix} 0 & k_x \\ -k_x & 0 \end{pmatrix}$$

$$\alpha_y^F = \begin{pmatrix} 0 & k_y \\ -k_y & 0 \end{pmatrix}$$

$$\alpha_z^F = \begin{pmatrix} 0 & k_z \\ -k_z & 0 \end{pmatrix}$$

which brings out more clearly the similarity in structure of the α 's with the ones that are contained in the Dirac equation for the four-spinor v . Therefore, it is not surprising that the k 's turn out to be nothing else but the r_x, r_y, r_z matrixas for infinitesimal rotations. As we know, the equivalence transformation that makes r_z diagonal changes r_x, r_y, r_z into v_x, v_y, v_z (except for the $\frac{\pi}{i}$ factor), i.e into the matrix elements of the angular momentum operator with eigenvalues $j=1$. Thus we can write (forgetting the $\frac{\pi}{i}$)

$$\alpha_i^F = \begin{pmatrix} 0 & v_i \\ -v_i & 0 \end{pmatrix}$$

which clearly shows the similarity with the α matrix for the four-spinor.

To obtain physical information from Dirac's equation, we make use of the relation defining the average value \bar{O} of an operator O :

$$\bar{O} \equiv \int (\mathbb{I}, O \mathbb{I}) d\mathbb{Z}$$

where the integral is performed over all volume and the brackets $()$ stand for the inner product in four spinor space.

We must expect the inner product of \mathbb{I} with itself to represent

the probability (as a function of space coordinates) of finding the electron at some point in space and therefore, that inner product multiplied by the electronic charge should give us the charge density, i.e:

$$\rho = e(\mathbb{I}, \mathbb{I}) = e \sum_{i=1}^4 |\Psi_i|^2$$

Using the continuity equation

$$\text{div } \mathbf{j} = -\dot{\rho}$$

we can show that the current density is:

$$\mathbf{j} = ec(\mathbb{F}, \underline{\alpha} \mathbb{F})$$

In the case of the electromagnetic field, the inner product of \mathbb{F} with itself should represent energy density u :

$$u = \frac{1}{8\pi} (\mathbb{F}, \mathbb{F})$$

The continuity equation for the electromagnetic field is:

$$\mathbf{i} = -\text{div } \underline{s}$$

where \underline{s} is the Poynting vector. We can also show that:

$$\underline{s} = -\frac{c}{8\pi} (\mathbb{F}, \underline{\alpha} \mathbb{F})$$

Quantization of the Radiation Field.

The electromagnetic field can be derived from a vector potential \underline{A} which satisfies the wave-equation in free space:

$$\square \underline{A} = 0 \quad (1)$$

If the time dependent part of the scalar potential is eliminated by a gauge transformation, then the transversality of electromagnetic waves is expressed by the divergence condition:

$$\text{div } \underline{A} = 0 \quad (2)$$

The electric and magnetic fields are given as follows:

$$\begin{aligned} \underline{E} &= -\frac{1}{c} \frac{\partial \underline{A}}{\partial t} \\ \underline{H} &= \text{rot } \underline{A} \end{aligned} \quad \left. \right\} \quad (3)$$

To quantize the radiation field it is first necessary to expand the vector potential as a linear combination of eigen-solutions of the equations (1) and (2). We confine the radiation field in a specified volume, and impose certain boundary conditions. This enables one to write any vector potential which obeys these boundary conditions as a linear combination of an infinite but denumerable number of orthogonal waves:

$$\underline{A} = \sum_{\lambda} \{ q_{\lambda}(t) \underline{A}_{\lambda}(\underline{r}) + q_{\lambda}^*(t) \underline{A}_{\lambda}^*(\underline{r}) \} \quad (4)$$

The index λ denotes the various quantum numbers which characterize each wave. It is convenient to normalize \underline{A}_{λ} so that:

$$\int_V \underline{A}_{\lambda}^*(\underline{r}) \cdot \underline{A}_{\lambda}(\underline{r}) d\underline{r} = 4\pi c^2 S_{\lambda\lambda} \quad (5)$$

where V is the enclosed volume. The \underline{A}_{λ} and their complex conjugates are solutions of the vector Helmholtz equation:

$$\Delta \underline{A}_{\lambda} + k_{\lambda}^2 \underline{A}_{\lambda} = 0 \quad (6)$$

(where k_{λ} is the wave number (an eigenvalue) characterizing \underline{A}_{λ} , and

of the divergence condition:

$$\text{div } \underline{A}_{\lambda} = 0 \quad (7)$$

Equations (6) and (7) can be combined to give a single "divergenceless vector Helmholtz equation"

$$\text{rot rot } \underline{A}_{\lambda} - k_{\lambda}^2 \underline{A}_{\lambda} = 0 \quad (8)$$

Any solution of eq. (8) automatically satisfies both of the two previous equations. The solutions of eq. (8) depend on the boundary conditions and will be discussed below. The field amplitudes q_{λ} (and q_{λ}^*) satisfy the harmonic oscillator equation:

$$\frac{d^2 q_{\lambda}}{dt^2} + \omega_{\lambda}^2 q_{\lambda} = 0 \quad (9)$$

where ω_{λ} is the frequency, equal to $c k_{\lambda}$.

Apart from a multiplicative constant and a harmonic time factor, the q_{λ} and q_{λ}^* represent annihilation and creation operators respectively. It is convenient to normalize these quantities so that the commutation rules obeyed by them are:

$$\begin{aligned} [q_{\lambda}, q_{\lambda}] &= [q_{\lambda}^*, q_{\lambda}^*] = 0 \\ [q_{\lambda}, q_{\lambda}^*] &= \frac{i\hbar}{2\omega_{\lambda}} \delta_{\lambda\lambda} \end{aligned} \quad \left. \right\} \quad (10)$$

The matrix elements of q_{λ} and q_{λ}^* taken between an initial state containing n_i quanta of type λ and a final containing n_f quanta of type λ are given by:

$$\begin{aligned} \langle n_{f,\lambda} | q_{\lambda} | n_{i,\lambda} \rangle &= \sqrt{\frac{n_{i,\lambda}}{2\omega_{\lambda}}} S_{n_f, n_{i,\lambda}} e^{-i\omega_{\lambda} t} \\ \langle n_{f,\lambda} | q_{\lambda}^* | n_{i,\lambda} \rangle &= \sqrt{\frac{(n_{i,\lambda}+1)}{2\omega_{\lambda}}} S_{n_f, n_{i,\lambda}+1} e^{i\omega_{\lambda} t} \end{aligned} \quad (11)$$

The Hamiltonian of the radiation field is given by:

$$H = \frac{1}{8\pi} \int_V \{ |\underline{E}|^2 + |\underline{H}|^2 \} dV \quad (12)$$

With the aid of eqs. (3), (4) and (5) this can be put into the form:

$$\mathcal{H} = \sum_{\lambda} 2\omega_{\lambda}^2 g_{\lambda}^* g_{\lambda} \quad (12)$$

The energy eigenvalues E_n are given by:

$$E_n = \sum_{\lambda} n_{\lambda} \omega_{\lambda} \quad (13)$$

The order of the field amplitudes g_{λ} and g_{λ}^* in eq. (12) has been chosen in such a way to give zero energy when no quanta are present.

Now, we want expand the vector potential in a series of standing spherical waves with a certain point O as center. This will result from choosing a sphere of large radius R_0 as volume of integration, with the boundary condition that the tangential components of \underline{A} vanish at the surface of the sphere. This is equivalent to confining the radiation field inside a sphere with a perfectly reflecting surface. The vector potential for each spherical wave decreases as r^{-1} for large distances r from the center, but remains finite throughout the volume of integration, and at center of the sphere. Each (standing) spherical wave has a definite angular momentum L and corresponds to the (outgoing) spherical wave emitted by a suitable oscillating classical 2nd pole located at O . (Cf. Blatt and Weisskopf). We could instead have quantized the radiation field into running plane waves by confining it within a cube and imposing the boundary condition that \underline{A} and its derivatives have the same values on opposite planes of this cube. (Cf. Heitler) However this approach, while simpler for most radiation problems of interest, is not well suited for a study of multipole radiation since plane waves do not carry a unique angular momentum, and since they do not correspond directly to the radiation emitted by a vibrating multipole.

The standing wave solutions of the equation (18), with boundary condition $A_{\text{tang}}(R_0) = 0$, can be expressed in terms of the solutions U_{LM} of the scalar Helmholtz equation:

$$\Delta u + k^2 u = 0$$

However, for each U_{LM} we can choose two linearly independent solutions $\underline{A}_{LM}^{\sigma}$, where σ is given the index "E" or "M" denoting electric or magnetic multipole fields. These solutions can be written as follows:

$$\begin{aligned} \underline{A}_{LM}^E &= \frac{i}{k_x} C_L \underline{\text{rot}} \underline{L} U_{LM} \\ \underline{A}_{LM}^M &= i C_L \underline{L} U_{LM} \end{aligned} \quad (14)$$

where $\underline{L} = -i \underline{r} \times \underline{\text{grad}}$ is the orbital angular momentum operator and C_L is an arbitrary constant and where:

$$\left[\frac{\partial}{\partial r} (\underline{r} U_{LM}) \right]_{R_0} = 0 \quad (15)$$

Each solution is understood to be also characterized by a k_x . Note that the solutions of (14) vanish identically for $L=0$. This is a consequence of the transverse nature of electromagnetic waves.

The $\underline{A}_{LM}^{\sigma}$ have the following properties:

- They form a complete orthogonal set of non-singular solutions to the divergenceless vector Helmholtz equation. Thus any vector function which does not have a singularity at the origin and whose tangential components vanish for $r=R_0$, can be expressed as some linear combination of the $\underline{A}_{LM}^{\sigma}$. The orthogonality condition for this case is:

$$\int_V (\underline{A}_{LM'}^{\sigma'})^* \cdot \underline{A}_{LM}^{\sigma} dV = \frac{\ell(\ell+1)}{2k_x^2} R_0 C_L^2 \delta_{\sigma\sigma'} \delta_{LL'} \delta_{MM'} \delta_{k_x k_x} \quad (16)$$

The normalization condition (5) is satisfied if:

$$C_L = \sqrt{\frac{8\pi \omega_x^2}{L(L+1) R_0}} \quad (17)$$

- The solutions $\underline{A}_{LM}^{\sigma}$ are eigenvectors of angular momentum operators (Strictly speaking, each of the three components of $\underline{A}_{LM}^{\sigma}$ is an eigenfunction). However, the total angular momentum is the sum of the orbital angular momentum \underline{L} and an intrinsic spin \underline{S} of

the radiation. Thus

$$\underline{J} = \underline{L} + \underline{S}$$

where \underline{S} is such that:

$$S_2 \underline{A} = i \underline{\epsilon}_z \times \underline{A}$$

where $\underline{\epsilon}_z$ is a unit vector in the z direction. Equations identical in form hold for the x and y components of \underline{S} .

The following equations can be derived:

$$\left. \begin{aligned} J_z \underline{A}_{LM}^{\sigma} &= M \underline{A}_{LM}^{\sigma} \\ J^2 \underline{A}_{LM}^{\sigma} &= L(L+1) \underline{A}_{LM}^{\sigma} \\ S^2 \underline{A}_{LM}^{\sigma} &= S(S+1) \underline{A}_{LM}^{\sigma} = 2 \underline{A}_{LM}^{\sigma} \end{aligned} \right\} \quad (18)$$

However $\underline{A}_{LM}^{\sigma}$ is not an eigenfunction of the operators:

$$L_z, L^2 \text{ and } S_z$$

These relations have the following physical interpretation:

The electromagnetic field which corresponds to a vector potential $\underline{A}_{LM}^{\sigma}$ contains total angular momentum L with component M in the z -direction. The radiation is also characterized by a spin 1. Indeed, it is easily shown from eqs. (13), (14) and (17) that the z -component of angular momentum:

$$\frac{1}{4\pi\hbar c} \int_V \underline{r} \times (\underline{E} \times \underline{H}) dV \quad (19)$$

of a single light quantum is equal to M , while the square of the angular momentum is $L(L+1)$

3) A characteristic feature of the vector potential $\underline{A}_{LM}^{\sigma}$ is its division into electric and magnetic multipoles. The electric and magnetic fields, \underline{E} and \underline{H} , are related to the vector potentials by:

$$\left. \begin{aligned} \underline{E}_{LM}^{\sigma} &= ik_x \underline{A}_{LM}^{\sigma} \\ \underline{H}_{LM}^{\sigma} &= \text{rot } \underline{A}_{LM}^{\sigma} \end{aligned} \right\} \quad (20)$$

(The time dependent part of these fields has been factored out as was done for the vector potential)

Note that:

$$\left. \begin{aligned} \underline{E}_{LM}^{\sigma} &= + \underline{H}_{LM}^M = i C_L \text{rot } \underline{L} \underline{U}_{LM} \\ \underline{E}_{LM}^M &= - \underline{H}_{LM}^{\sigma} = - k_x C_L \underline{L} \underline{U}_{LM} \end{aligned} \right\} \quad (21)$$

These fields satisfy the following equations:

$$\underline{r} \cdot \underline{E}_{LM}^{\sigma} = \underline{r} \cdot \underline{H}_{LM}^{\sigma} = 0 \quad (22)$$

i.e. an electric multipole field has non-vanishing radial components of the electric field \underline{E} but not of the magnetic field \underline{H} , while a magnetic multipole field has non-vanishing radial components of \underline{H} , but not of \underline{E} .

The two solutions $\underline{A}_{LM}^{\sigma}$ and \underline{A}_{LM}^M have opposite parity, namely $(-)^{L-1}$ and $(-)^L$, respectively. The parity of the radiation field itself is opposite to the parity of the vector potential. Thus an EL or ML radiation field carries parity $(-)^L$ or $(-)^{L-1}$, respectively. In any case, a knowledge of k_x , L , M and parity of the vector potential $\underline{A}_{LM}^{\sigma}$ uniquely specifies its form.

On the Theory of Fundamental Interactions.

Introduction: (J. Schwinger, Annals of Phys., 2, 407, 1957)

The great problem facing Physics today is that of classifying the numerous particles - known or anticipated - within a general scheme. We must explain why these particles exist and no others: i.e. we must explain and predict their mass spectra and their charge and spin properties. Also we must understand the various roles played by interactions of different orders of strength, and the relation of these to the broad conservation laws of Physics.

The division of particles into two great statistical categories is generally accepted. Heavy bosons and heavy fermions have strong interactions between them. Transitions under strong interaction correspond to a time scale of the order t/Mc^2 , M being the nucleon mass, i.e. 10^{-24} sec. The intermediate electromagnetic interaction is characterized by the fine-structure constant and corresponds to a time-scale 100 times longer i.e. is of order 10^{-22} sec. The weak interactions are responsible for non-electromagnetic decays and correspond to a time-scale of around 10^{-10} sec, roughly the lifetime of hyperons and K-mesons. Over the long period all particles decay into the stable N^+, e, ν (or their antiparticles) and γ . Note that the decay products of any one heavy Fermion always include another. The number of heavy fermions is conserved for strong interactions. If, in order to allow for pair creation and annihilation, we make the assignment ± 1 to heavy fermions and their antiparticles resp., the sum of the numbers assigned - the so-called baryon number - is conserved. The light particles are decay products of weak or intermediate interactions. The only stable boson is the photon.

In addition to the gross mass-spectrum there is in general a fine-structure splitting between charged and neutral particles. The EM interaction is a physical agency which destroys a kind

of symmetry that would exist in its absence, in the sense that it distinguishes between charged and neutral particles. We infer that the physical reason for the mass fine-structure lies with the E-M field, by which is meant that in a hypothetical world in which this field does not exist these particles would be absolutely indistinguishable.

In an experiment extended over a time of 10^{-22} sec, one would then begin to distinguish neutron from proton and π^+ from π^0 by their associated mass differences. In the same way the much larger mass differences occurring in the heavy fermion group might be resolved by postulating some very strong interaction in whose absence hyperons would be absolutely indistinguishable from the proton. For such an interaction distinction of the particles becomes possible within 10^{-24} sec., earlier than in the E.M. case. In a hypothetical world in which the weak interactions, the EM int. and this strong int. which we have yet to identify have all been turned off, the hyperons coalesce into a super multiplet of a kind of higher inner multiplicity which is actually brought into physical existence by a succession of interactions.

It is to be expected that the weak int. give rise to small mass fine-structure. However, since they are responsible for decays they introduce a different kind of mass connection: an analytic way of representing this decay degeneracy is to say that the masses of the particles which decay are complex. When the weak interactions come into play there is the final breaking down of symmetry and we are left with a few stable end particles.

This is the sort of general programme at which we might aim: proceeding from the familiar weak int. to the EM int. to others of increasing strength, trying always to reduce the multiplets occurring at each stage to a singular single particle whose inherent multiplicity is exhibited by weaker int. coming into play. The experiments suggest that the longer the time-scale the more approx. the conservation laws become. Apart from the usual space-time quantities: energy, spin,

etc. The only properties of these particles that are exactly conserved are: 1) the electric charge, representing the exact stability of electron and positron, and 2) the baryon number of nucleons, representing the exact stability of the proton.

The problem cannot be solved on the basis of familiar space-time properties, in particular spin. The experimental evidence is altogether consistent with the belief that all fermions have spin $\frac{1}{2}$ and that the boson spins are restricted to the two possibilities 0 and 1. In the QT of F these spin values are not only distinguished by simplicity but are also the only ones that allow consistent development. In each case we have to construct a field possessing multiplicities over and above the usual space-time ones and corresponding to internal degrees of freedom realizable through various interactions. The fields are coupled through the interactions which occur in a particular sequence and each one of which is characterized by a certain symmetry-destroying property. The interaction of lowest symmetry, the weak interaction which allows the particles to decay into each other, occurs last in the sequence, leaving finally only those particles which are distinguishable on the basis of space-time properties alone properties which are therefore always exactly conserved.

Quantum Theory of Fields

The problem of the mathematical description of the particles is expressed in terms of the language of quantum field theory. Quantum field theory is the ultimate expression of the particle-wave duality or of the complementarity which exists between the classical concepts of particle and field. The QT of F is in fact a kind of union of the two principles of complementarity on the one hand and relativity on the other. It is the finest expression that we have of the requirements that must be satisfied by any physical theory. Although this theory is not complete, it is the only recourse

available at present for the relativistic treatment of particles and fields.

We will not follow the conventional way of developing the subject. The conventional method takes a classical system and promotes it to a quantum mechanical system. In doing this, one had to be given the classical analogue. Not all attributes of physical particles can be given in this way, e.g. the spin of the electron, so that this procedure is at best incomplete and unsatisfactory in a physical sense. Further, to get a description of a Fermi-Dirac field, one artificially had to change commutation relations into anticommutation relations. The correspondence principle procedure for quantizing the fields thus introduces an artificial asymmetry between the treatments of the two fundamental types of fields since only one of these, the Bose-Einstein case, has a classical analogue. This is the first objection to the usual quantization procedure. The second objection is directed against the use of the Hamiltonian formalism where commutation relations are artificially imposed on the canonical variables. Thus the usual methods of quantization based on the classical analogies and the Hamiltonian formalism are not adequate when one wants to deal with a comprehensive theory of fields.

The first task is to banish the correspondence principle from the QT of F. because the systems to be dealt with, lie far beyond the domain for which it was intended. The second is to find a dynamical description which is manifestly covariant. We will present a formulation of quantum dynamics entirely self-contained, i.e. independent of classical analogies and based on a Lagrangian which is relativistic invariant.

For simplicity a system with a finite number of freedom is dealt with. All important features of the theory will become apparent here. The usual quantum mechanical concepts of states and observables are assumed. A state characterized by the maximum number of physically compatible observables a_i at time t is represented by right and left vectors $|a_i, t\rangle$ or $\langle a'_i, t|$ respectively. The set of states form a Hilbert space and physical quantities are represented by operators X which act

on the vectors representing the states.

An important concept is the notion of equivalent descriptions of states. To any vector $\langle 1 |$ representing a state there corresponds another vector

$$\overline{\langle 1} = \langle 1 | U$$

where U is a unitary operator

$$U^\dagger U = 1$$

Similarly $\overline{\langle 1} = U^{-1} \langle 1 |$

and $\overline{| X \rangle} = U^{-1} | X \rangle$

The barred quantities form an equivalent description of the states and observables represented by $\langle 1 |, | 1 \rangle$ and $| X \rangle$. The equivalence is a consequence of the fact that all algebraic relations between vectors and operators are preserved under unitary transf.

Since all unitary transf. can be built up by a successive application of infinit. unitary transf., a study of the latter is adequate and particularly important. Consider

$$U = 1 + iG$$

where G is an infinit. and Hermitian generator. The changes induced by such a transf. are:

$$\delta \langle 1 | = \overline{\langle 1} - \langle 1 | = \langle 1 | iG$$

$$\delta | X \rangle = -iG| X \rangle$$

$$\delta | X \rangle = | X \rangle - \overline{| X \rangle} = \frac{1}{i} [| X \rangle, G]$$

where $[| X \rangle, G] = | X \rangle G - G | X \rangle$. Notice that for later convenience the usual def. of the sign of $\delta | X \rangle$ has been reversed.

The purpose of the quantum dynamics is to find the relations between a state $\langle a'_1, t_1 |$ of a system at a certain time t_1 and the state $\langle a'_2, t_2 |$ at another time t_2 . All the information about the dynamical relationships is contained in the transf. funct. $\langle a'_1, t_1 | a'_2, t_2 |$. There are two principal ways of constructing such a function. One way, due to Feynman, gives an explicit rule of construction by means of an integral formulation. This way suffers from the objection that the nature of the dynamical

variables, i.e. Fermi-Dirac or Bos-Einstein, has to be prescribed and is not a consequence of the formulation itself. The other way, to be used here, allows us to discover automatically that there are two kinds of fields and two only. This method may be characterized as the differential formulation.

The differential method specifies not the transf. funct. itself, but the inf. change in the transf. funct. when anything in the nature of the system is altered. Thus, a differential eq. is obtained, the integration of which leads to the transf. function.

Many kinds of infinit. changes can be envisaged. The initial and final states, the time of reference, physical properties, and the dynamical nature, e.g. mass, are quantities that can be varied. Any infinit. change of the transf. function can be represented by:

$$\delta \langle a'_1, t_1 | a'_2, t_2 | = i \langle a'_1, t_1 | S W_{12} | a'_2, t_2 |$$

This is merely the definition of the operator $S W_{12}$. a'_1 represents a complete set of commuting Hermitian op. a'_2 may be either the same or a different set. The reality property:

$$\langle a'_1 t_1 | a'_2 t_2 |^* = \langle a'_2 t_2 | a'_1 t_1 |$$

of the transf. function implies that

$$S W_{12}^+ = S W_{12}$$

and the composition law:

$$\langle a'_1 t_1 | a'_3 t_3 | = \sum_{a'_2} \langle a'_1 t_1 | a'_2 t_2 | \langle a'_2 t_2 | a'_3 t_3 |$$

implies the additivity of the infinit. transf. under comp. Thus:

$$S W_{13} = S W_{12} + S W_{23}$$

The basic postulate of the dynamical principle is that there exists a certain class of alterations for which the associated operators $S W_{12}$ are obtained by appropriate variations of a single operator

$$SW_{12} = S(W_{12})$$

where W_{12} is called the action operator (This is a pure number). Plank's const. \hbar arises in a natural way when we want to identify this (microscopic) action with the action of the macroscopic dynamics. Another way of expressing the same thing is to say that we have here chosen the units such that $\hbar = 1$). The reality and composition properties of SW_{12} imply:

$$W_{12}^\dagger = W_{12}$$

$$W_{12} + W_{23} = W_{13}$$

The transf. funct. reduces to a constant number if the set a_1 is the same as a_2 and $t_1 = t_2$. Thus:

$$S\langle a', t+a'', t \rangle = S(a' - a'')$$

Hence the variation of time gives:

$$S\langle a', t+a'', t \rangle = 0$$

This together with the additivity prop. shows that the action operator must possess the form:

$$W_{12} = \int_{t_2}^{t_1} dt L(t) \quad (1)$$

where $L(t)$ is a hermitian function of the dynamical variables $\chi_a(t)$, $a = 1, \dots, n$. With no loss of generality the χ_a may be required to be hermitian.

For a given dynamical system the times t_1 and t_2 as well as the dynamical variables χ_a may be varied. This corresponds to the possibility of introducing infinit. changes in the transf. functions, i.e. either infinit. alterations of the complete set of operators or of the times to which they refer. The variations are localized at the times t_1 and t_2 since the history of the system is fixed between these times. Hence:

$$S\langle a'_1, t_1 \rangle = i \langle a'_1 | t_1 | G_1 \rangle$$

$$S\langle a'_2, t_2 \rangle = -i G_2 | a'_2 | t_2 \rangle$$

where G_1 and G_2 are infinit. hermitian op. funct. of the variables at t_1 and t_2 respectively. The above relations imply:

$$S\langle 1 \rangle = i \langle | G_1 - G_2 | \rangle$$

$$\text{and: } SW_{12} = S \int_{t_1}^{t_2} dt L(t) = G_1 - G_2$$

This is the quantum mechanical form of Hamilton's principle, the principle of stationary action.

Note that two lagrangians differing by a time derivative describe the same system. Thus:

$$\bar{L} = L - \frac{d}{dt} W \quad W = W(\chi, t)$$

yields:

$$\bar{W}_{12} = W_{12} - (W_1 - W_2)$$

Therefore the action principle for \bar{W}_{12} is satisfied if it is satisfied by W_{12} . That is, W_{12} and \bar{W}_{12} imply the same eq. of motion but

$$S\bar{W}_{12} = \bar{G}_1 - \bar{G}_2$$

$$\text{where: } SW_1 = G_1 - \bar{G}_1 \quad \text{and } SW_2 = G_2 - \bar{G}_2$$

Note also that since the lagrangian is local in time, as demanded by the additivity condition, the equations of motion will be differential equations of finite order. These can be arranged as a set of first order eqs. and hence the lagrangian is deliberately chosen to yield first order eqs. Thus it must possess the form:

$$\begin{aligned} L &= \frac{1}{4} \sum_{a,b} \left(\chi_a A_{ab} \frac{d\chi_b}{dt} - \frac{d\chi_a}{dt} A_{ab} \chi_b \right) - H(\chi, t) = \\ &= \frac{1}{4} (\chi A \frac{d\chi}{dt} - \frac{d\chi}{dt} A \chi) - H \end{aligned} \quad (2)$$

The time derivative term has been symmetrized with respect to the operation of integration by parts, corresponding to the freedom of adding a time derivative to the lagrangian. If L is to be a hermitian operator this property must apply to H , the hamiltonian

operator and the numerical matrix A must be skew-hermitian, i.e.
 $A^+ = -A$.

The action operator is:

$$W_{12} = \int_{t_2}^{t_1} \left[\frac{1}{4} (\chi A dx - d\chi A \chi) - H dt \right]$$

In order to vary the time an auxiliary variable τ can be introduced such that variations δt_1 and δt_2 are represented by a change in the functional dependence of t upon τ . This enables us to vary the x_α and t with fixed limits z_1 and z_2 . The auxiliary variable need not be written explicitly since it is not subject to variation. Hence

$$\begin{aligned} \delta W_{12} = & \left[\left[\frac{1}{2} (\delta \chi A dx - d\chi A \delta \chi) - \delta H dt + dH \delta t \right] \right. \\ & \left. + \int d \left[\frac{1}{4} (\chi A \delta \chi - \delta \chi A \chi) - H \delta t \right] \right] \end{aligned}$$

The action principle asserts that

$$\frac{1}{2} (\delta \chi A dx - d\chi A \delta \chi) = \delta H dt - dH \delta t$$

$$\text{or: } \delta H = \frac{dH}{dt} \delta t + \frac{1}{2} [\delta \chi A \frac{dx}{dt} - \frac{dx}{dt} A \delta \chi] \quad (3)$$

the equations of motion, and further that

$$G = \frac{1}{4} (\chi A \delta \chi - \delta \chi A \chi) - H \delta t \quad (4)$$

at times t_1 and t_2 .

The Hamiltonian operator is an arbitrary function of the x_α . If its variation is to possess the form (3) with δx_α appearing only on the left or on the right, these variations must possess elementary operator properties characterizing the class of variations to which the dynamical principle ~~refers~~ refers. Thus one should be able to displace δx_α entirely to the left, or to the right, in the structure of δH . Thus:

$$\delta H - \frac{\partial H}{\partial t} \delta t = \delta \chi \frac{\partial eH}{\partial x} = \frac{\partial rH}{\partial x} \delta \chi$$

These eqs. define the left and right derivatives of H .

The complete symmetry between left and right in the multiplication allows one to infer that the terms in (4) with $\delta \chi$ on the left and on the right, are in fact equal. Thus one obtains.

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} \quad (5a)$$

$$\text{and: } A \frac{dx}{dt} = \frac{\partial eH}{\partial x} \quad (5b)$$

$$- \frac{dx}{dt} A = - A^T \frac{dx}{dt} = \frac{\partial rH}{\partial x} \quad (5c)$$

where the latter must be equivalent forms of the equations of motion. Similarly

$$G = -\frac{1}{2} \delta \chi A \chi - H \delta t$$

$$\text{and } G = \frac{1}{2} \chi A \delta \chi - H \delta t = \frac{1}{2} (A^T \chi) \delta \chi - H \delta t$$

must be equivalent forms of the infinit. generator G . G is conveniently split into two parts:

$$G = G_x + G_t$$

$$\text{where: } G_t = -H \delta t \quad (6a)$$

$$\text{and: } G_x = \frac{1}{2} \chi A \delta \chi = -\frac{1}{2} \delta \chi A \chi \quad (6b)$$

G_t is the infinitesimal generator of a time variation. G_x is the infinit. generator of the variables x_α at a given t .

We have two different forms of the eq. of motion, one involving the matrix A and one involving A^T . In general a consistent theory, without undue restrictions on the structure of the Hamiltonian, will be obtained only if the matrix A is completely reduced under the operation of transposition, i.e. if A^T does not differ fundamentally from A . That is to say that A must be completely reduced into two submatrices a and χ :

$$A \sim \begin{pmatrix} a & 0 \\ 0 & \chi \end{pmatrix}$$

in which a is antisymmetric and χ symmetric. From this cond. and

The previous prop. of A one obtains:

$$a = -a^T = a^*$$

$$\alpha = \alpha^T = -\alpha^*$$

The corresponding decomposition of the χ_a yields two kinematically independent sets of dynamical variables: variables of the first kind z , associated with a , and variables of the second kind \bar{z} , associated with α . We find, using the esp. forms of a and α , that G_x decomposes to $G_z + G_{\bar{z}}$ where

$$G_z = \frac{1}{2} z (a \delta z) = \frac{1}{2} (a \delta z) z$$

$$G_{\bar{z}} = \frac{1}{2} \bar{z} (\alpha \delta \bar{z}) = -\frac{1}{2} (\alpha \delta \bar{z}) \bar{z}$$

from which it is evident that the variations δz , $\delta \bar{z}$ satisfy the relations:

$$[\delta z_i, z_j] = \{\delta \bar{z}_k, \bar{z}_l\} = 0$$

where:

$$[A, B] = AB - BA \quad \{A, B\} = AB + BA$$

The kinematic indep. of the sets of variables z and \bar{z} implies that:

$$[\delta z_i, \bar{z}_j] = [\delta \bar{z}_k, z_l] = 0$$

We have, in these operator properties of the variations δz and $\delta \bar{z}$ the precise specifications of the class of variations to which the fundamental dynamical principle refers.

In accordance with the decomposition of A, the Lagrangian becomes:

$$L = \frac{1}{4} \{ z, a \frac{dz}{dt} \} + \frac{1}{4} \{ \bar{z}, \alpha \frac{d\bar{z}}{dt} \} - H$$

The symm. or antisymmetrization indicated by the brackets will henceforth be denoted by dots, viz.:

$$L = \frac{1}{2} z \cdot a \frac{dz}{dt} + \frac{1}{2} \bar{z} \cdot \alpha \frac{d\bar{z}}{dt} - H \quad (17)$$

where the diff. interpretation of the dot corresponds to the kind

of variable involved. The eqs. of motion become:

$$a \frac{dz}{dt} = \frac{\partial H}{\partial z} = \frac{\partial r H}{\partial z}$$

$$\alpha \frac{d\bar{z}}{dt} = \frac{\partial H}{\partial \bar{z}} = \frac{\partial r H}{\partial \bar{z}}$$

Since δz anticommutes with \bar{z} , the opposite signs of the left and right derivatives of H with respect to z imply that H must be an even function of the z .

G_z and $G_{\bar{z}}$ lead also to the commut. rel. of the variables themselves. But let consider G_t . If F is some function $F(\chi(t), t)$ obtained by replacing $\chi(t)$ by $\chi(t+St)$ without altering the explicit dependence of F on t , viz.:

$$\bar{F} = F + \left(\frac{dF}{dt} - \frac{\partial F}{\partial t} \right) St$$

The general relation:

$$\delta F = F - \bar{F} = \frac{1}{i} [F, G]$$

therefore yields:

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{1}{i} [F, H] \quad (18)$$

This is the usual Heisenberg form of the eqs. of motion, if we consider H to be the energy operator. For this reason $-H$ will be called the dynamical part of L and the remainder the kinematical part.

Now:

$$\begin{aligned} \frac{1}{i} [F_G, H] &= -\frac{1}{i} \left[\frac{1}{2} \delta X A Y, H \right] = -\frac{\delta Y}{2i} [A X, H] = -\frac{1}{2} \delta Y A \frac{dX}{dt} = \\ &= -\frac{1}{2} \delta X \frac{\partial H}{\partial X} \end{aligned}$$

where we have used eqs. (16) and (18) as well the fact that δX commutes with H . It follows from the df. of the left derivative that G_X generates a change $\frac{1}{i} \delta X$ in the variable X . The commutation rel. of the χ_a was follows from applying G_z and $G_{\bar{z}}$ in turn, viz.:

$$\frac{1}{i} [z_i, \frac{1}{2}(a\delta z)z] = \frac{1}{2} S z_i$$

(9a)

$$\frac{1}{i} [\bar{z}_k, \frac{1}{2}(\alpha\delta \bar{z})\bar{z}] = \frac{1}{2} S \bar{z}_k$$

(9b)

from which with the aid of the comm. rel. of the variations $\delta z, \delta \bar{z}$ we obtain:

$$[z_i, z_j] = i(a^{-1})_{ij}$$

$$\{\bar{z}_k, \bar{z}_l\} = i(\alpha^{-1})_{kl}$$

(9a)

(9b)

while kinematic ineq. insures that:

$$[z_i, \bar{z}_k] = 0$$

(9c)

The non-singularity of a and α is of course implied in the decoupl. procedure. As a general requirement of consist. it can be shown (Cf. Schrödinger Phil Mag Vol. 44 p. 1171) that both matrices must be of even order, i.e. that the number of variables of each kind must be even. Finally the eq. (9b) shows that the matrix must be positive-definite. The familiar Heisenberg commut. rel. result for the variables of the first kind when the canonical form of the matrix a is employed.

In generalizing the foregoing to the description of fields, the employment of the Lagrangian rather than the Hamiltonian as the basis of quantization not only leads to a manifestly covariant theory but also introduces automatically two types of field variables corresponding to the statistical division of elementary particles: Fermi-Dirac and Bose-Einstein fields appear simultaneously. This will simplify later discussion of the various kinds of interaction symmetry exhibited by the fields and help in constructing the hierarchy of interactions. A field is described by a finite number of functions $\chi_{\alpha}(x)$, where x denotes collectively the four space-time coordinates which must clearly now appear on the same footing. The notion of compatibility of measurements at a particular time, required in

our previous definition of a state, can now be generalized to space-like surfaces, i.e. surfaces any two of whose points are separated by a space-like vector and which cannot therefore be connected by signals. States now consist of a complete set of compatible measurements carried out on such a surface, and are represented by vectors $|a' \tau_1\rangle$ and $|a' \tau_2\rangle$ expressing the non-influence of measurements a' performed at points of any given space-like surface τ . We set $c = \hbar = 1$ and choose as metric tensor:

$$g^{\mu\nu} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

Thus:

$$X^\mu X_\mu = X^2 - X_0^2 \begin{cases} > 0 & \text{if } X^\mu \text{ space-like} \\ < 0 & \text{if } X^\mu \text{ time-like.} \end{cases}$$

The fundamental dynamical principle becomes:

$$S\langle a' \tau_1 | a' \tau_2 \rangle = i \langle a' \tau_1 | \delta W_{12} | a' \tau_2 \rangle$$

where the reality and composition properties of δW_{12} require the form:

$$W_{12} = \int_{\tau_1}^{\tau_2} d^4x \mathcal{L}[x]$$

\mathcal{L} being the hermitian field lagrangian. The special class of variations to which the principle refers may be established as before. Again:

$$\delta W_{12} = G_1 - G_2$$

G_1 and G_2 depending exclusively upon the surfaces τ_1, τ_2 resp. By analogy the χ_α are assumed hermitian. The generalized lag. is:

$$\mathcal{L} = \frac{1}{4} [K A^M \partial_\mu X - \partial_\mu X A^M] - \mathcal{H}(X) \quad (10)$$

where the appearance of all four space-time derivatives, required for covariance, gives rise to four skew-hermitian matrices A^M .

\mathcal{L} is chosen to yield first order field eqs. The equivalence of the two forms:

$$A^\mu \partial_\mu \chi = \frac{\partial \mathcal{L}}{\partial \chi}$$

and:

$$-A^{\mu T} \partial_\mu \chi = \frac{\partial \mathcal{L}}{\partial \dot{\chi}}$$

demands the simultaneous reduction of the A^μ , while the χ_a reduce additively to boson fields ϕ and fermion fields ψ .

There is now an added freedom in the choice of variations, since the space-time co-ordinates can be varied within the region of integration quite apart from the variation of the χ_a , yielding:

$$G = G_x + G_\chi$$

G_χ being the covariant generalization of $-H\delta t$. It is to be expected that

$$G_\chi = S X^\mu P_\mu$$

where P_μ is the field energy-momentum vector. Similarly, if rotations $S\Omega^{\mu\nu}$ are considered the resulting form of G_χ is:

$$G_\chi = \frac{1}{2} S \Omega^{\mu\nu} J_{\mu\nu}$$

$J_{\mu\nu}$ being the field angular-momentum tensor (Cf. Schwinger Phys Rev 91, 3 p. 713). Turning instead to G_x note that

$$S L = \frac{1}{4} [X A^\mu \partial_\mu \delta X - \partial_\mu \delta X A^\mu X] + \frac{1}{4} \partial_\mu [X A^\mu \delta X - \delta X A^\mu X] \delta X$$

the divergence term resulting from int. by parts. Thus:

$$G_\chi = \int d\sigma_\mu \frac{1}{4} [X A^\mu \delta X - \delta X A^\mu X]$$

$d\sigma_\mu$ being a three-dim surface element of spacetime directed along the normal drawn outward from the region of integration. Now a space-like surface possesses the prop. that a special coordinate syst. exists in which it consists of all space at a particular time. In this special coordinate syst:

$$G_\chi = \int d^3x \frac{1}{4} (X A^0 \delta X - \delta X A^0 X)$$

This shows that A^0 takes a special place in the formalism; in particular it must in general be chosen non-zero, and if it is not, the field eqs. contain subsidiary rel. among the X_a .

Fermion fields of spin $\frac{1}{2}$ can be described by the Lagrangian:

$$\mathcal{L}^{(\frac{1}{2})} = -\frac{1}{2} [\psi \cdot \beta \gamma^\mu \frac{1}{i} \partial_\mu \psi + m_0 \psi \cdot \beta \bar{\psi}]$$

The hermitian functions ψ are four in number and are field variables of the 2nd kind. In accordance with their definition, the dots indicate symmetrisation with a factor $\frac{1}{2}$. The 4×4 matrices β , γ^μ satisfy:

$$\beta^2 = 1 \quad \text{p. antisymmetric and imaginary.}$$

$$(\gamma^\mu)^2 = -1 \quad \gamma^\mu \text{ sym. and imaginary.}$$

$$\{\gamma^\mu, \gamma^\nu\} = -2g^{\mu\nu} \quad \gamma^0 = \beta$$

The requirements for a description of variables of the 2nd kind are clearly satisfied (of the matrix α discussed earlier) The field eqs. are:

$$(\frac{1}{i} \gamma^\mu \partial_\mu + m_0) \psi = 0$$

The use of hermitian ψ is essentially the Majorana description of the Dirac electron theory (E. Majorana N. Cimento 14, p. 171, 1937) it allows the insertion of internal degrees of freedom at a later stage.

Boson fields of spin 0 can be described by 1st order eqs. if a five component representation (φ, φ^M) is employed: (φ^M = transverse)

$$\mathcal{L}^{(1)} = -\frac{1}{2} [\dot{\varphi}^\lambda \cdot \partial_\lambda \varphi - \dot{\varphi}^\lambda \partial_\lambda \varphi^\lambda - \dot{\varphi}^\lambda \partial_\lambda \varphi^\lambda + \mu_0^2 \varphi^2]$$

where the dot notation now implies antisymm. with a factor $\frac{1}{2}$, and the five components of φ, φ^M are as usual chosen to be hermitian. The field eqs. are:

$$\partial_\lambda \varphi^\lambda = \dot{\varphi}_\lambda \quad \partial_\lambda \varphi^\lambda = \mu_0^2 \varphi$$

from which the Klein-Gordon eq.

$$\square \phi = \mu^2 \phi$$

is readily recovered. Note that the field eqs. involve time derivatives of only two of the five components, namely ϕ and ϕ^0 . As a result, the variations of the other three are determined by the variations of these. ϕ and ϕ^0 are the only two indep. comp.

The comm. rel. arise on the application of the action principle from the inf. generators which describe changes of the field on the boundaries. Those infint. generators come by partial int. from derivations of the variations. For $\dot{\tau}$ the generator would be in the form:

$$G\dot{\tau} = \int d\sigma \mu \frac{i}{2} \delta \gamma^M S\dot{\tau}$$

If σ_μ has a time like direction, in some suitable coordinate syst. we obtain:

$$G\dot{\tau} = \int d\sigma i + \phi^0 \frac{S\dot{\tau}}{2}$$

This is the generator of transf. by which the field $\dot{\tau}$ is changed by an amount $\frac{1}{2} S\dot{\tau}$. The generator is a sum of contributions from all space at a given time. The additive term corresponds to the dynamical independence of the field at different space points at the same time. So:

$$[\dot{\tau}(x), G] = \frac{i}{2} S\dot{\tau}(x) = i[\dot{\tau}(x), \int d\sigma' \dot{\tau}(x') \delta \gamma^0 \frac{S\dot{\tau}(x')}{2}]$$

Making use of the fact that this is a system of 2nd kind where $S\dot{\tau}$ anticommutes with all the other operators, we obtain:

$$\frac{i}{2} S\dot{\tau}(x) = i \int d\sigma' [\dot{\tau}(x) \dot{\tau}(x') \delta \gamma_0 + \dot{\tau}(x') \delta \gamma_0 \dot{\tau}(x)] \frac{S\dot{\tau}(x')}{2}$$

$$\text{Thus: } \{\dot{\tau}(x), \dot{\tau}(x')\} = \delta(x-x')$$

when we recall that $\delta \gamma^0 = 1$ and $\delta(x-x')$ is a three dim. δ function

for the Bose field the corresp. generator is

Now the $\dot{\tau}(x)$ are hermitian op., and thus the comm. rel. is expressed by a positive definite symm. product. This positive definiteness depends upon the positive definiteness of the product $\beta \gamma_0$, i.e. there is a requirement of consistency for a F-D field. The matrix which appears in connection with the time derivative in the Lagrangian will appear in the commut. rel. and the above choice of sign in the lag. requires this matrix to be posit. def.

For the Bose field the corresp. generator is:

$$G\dot{\phi} = \int d\sigma \mu \frac{1}{2} [\phi \delta \gamma^M - \gamma^M \delta \phi]$$

Again in a suitable coordinate system this simplifies to:

$$G\dot{\phi} = \int d\sigma \frac{1}{2} [\phi \delta \phi^0 - \phi^0 \delta \phi]$$

Here we can observe the degenerate possibilities which are in fact the usual situation. The field has five components ϕ, ϕ^0 . In the generator only two of those components appear, i.e. $\phi, \delta \phi^0$. Thus only two components can be subjected to independent variation and on referring to the eqs. of motion, one sees that the time derivative appears only for ϕ and ϕ^0 , e.g.:

$$\partial_\mu \phi = \phi_\mu \quad \partial_\mu \phi^0 = \mu^2 \phi$$

The time derivative does not appear in the 1,2,3 components of the 1st eq. These eqs. determine ϕ_1, ϕ_2, ϕ_3 at a given time when ϕ is given. Thus ϕ_1, ϕ_2, ϕ_3 are not independent.

Bearing this in mind one proceeds to find comm. rel. from the generator $G\dot{\phi}$ as before. In this case ϕ is a field of the 1st kind so that $S\phi$ comm. with all the op. Then

$$[\phi(x), \phi(x')] = 0$$

$$[\phi^0(x), \phi^0(x')] = 0$$

$$[\phi(x), \phi^0(x')] = -i \delta(x-x')$$

The arguments of the functions refer to different space points at the same time. The comm. rules for ϕ_1, ϕ_2, ϕ_3 can be obtained from these

by taking space derivatives.

From the Lagrange function the structure of the energy operator can be obtained.

$$P^0 = \int d\sigma \frac{1}{2} [\varphi^0{}^2 + \sum_k (\varphi^k)^2 + \mu_0^2 \varphi^2]$$

This is the generator of a time displacement and may be obtained by removing from the Lagrangian those parts containing time derivatives. What is left is the energy operator. For a B-E syst. this op. must be positive definite. If the energy were not posit. def. one could have the non-phys. possibility of a syst with arbitrary low energy. This follows from the fact that for a B-E syst. there is no limit to the number of particles which can be put into a state.

Here again is a requirement of posit. definiteness. In the Fermi case it was in the nature of the comm. rel.; in the Box case, in the structure of the energy operator.

Consider a general Fermi field ψ with higher inner multiplicity. One has: 4 × multiplicity = number of components of ψ .

Similarly for the Box case one can introduce φ : 1 × multiplicity = number of comp. of φ .

We are now thinking very explicitly of the strongly interacting particles, the nucleons and hyperons which we believe are related to a fundamental field ψ out of which they have become physically distinguishable by distinguishing the various internal degrees of freedom. A similar situation is believed to exist for the spin 0 fields.

The Lagrange function now takes the form:

$$\mathcal{L} = \frac{1}{4} (\psi A^\mu \partial_\mu \psi - \partial_\mu \psi A^\mu) - \mathcal{H}(\psi)$$

where ψ is a field with some inner multiplicity and the A^μ are matrices which may describe both spin properties and prop. involving the multiplicity which go beyond space time properties.

If there is a part in A^μ referring to the internal space, multiplying the spin parts, then by a previous argument it also must be a

a positive definite matrix, for both the F-D field on the one hand and for the B-E field on the other. In this case, it may be absorbed into the definition of the generalized ψ field and one may say that the matrices A^μ refer only to space-time prop and not to the internal prop.

If we have internal prop, these fields are in a space which is the product of a spin space and an internal space which gives the mult. beyond the space time prop. Also, we must have the freedom of performing transf. in this internal space in order to exhibit the hierarchy of particles and their interactions as a successive break down of symm. prop. We want to find out something about the structure of the group that describes the transf. in the internal space. If we have the possibility of such transf. under the Lag. function is at least potentially invariant the kinematical term must be invariant. Whether the complete Lag. is invar or not will depend on the nature of the invariance of the general dynamical term \mathcal{H} . The point is that the possibility of admitting the group at all depends on the general invariance of the kinematical term which refers only to the kinds of degrees of freedom and not at all to the dynamics.

In this case we must have the possibility of replacing the set of fields ψ by a new set which are linear combination of the original one, i.e. $\tilde{\psi}(x) = \Lambda \psi(x)$ where Λ is a finite dim. matrix acting only on the internal degrees of freedom. This must be an invariant transf. at least for the kinematical term. Λ must be real because the field are hermitian. Also, since A^μ does not refer to the internal prop. and the kinematical term is considered invar, one has

$$\Lambda^\dagger \Lambda = 1$$

We are particularly interested in those groups which possess infinit. generators. Therefore let us assume:

$$\Lambda = 1 + i S W T$$

where δw is real and infinit. The cond. on Λ imply and

$$T^T = -T$$

$$T^* = -T$$

$\therefore T$ is hermitian.

If the dynamical term as well as the kinematical term is invariant we are dealing with an exact invariance principle and we wish to see to what this corresponds in terms of physical prop.

To do this let us apply a transf. of this type to the action principle. Then:

$$\bar{\chi} = (1 + i\delta w T) \chi = \chi - \delta \chi$$

$$\delta_T \chi = -i \delta w T \chi$$

where δw is a number.

Suppose this leaves the Lagrange function invar, i.e $\bar{L} = L$, and consider a generalization where δw is made a function of position and time but remains constant on the boundaries. This corresponds to choosing different linear comb. of fields at diff. places and diff. times in a continuous fashion. Then:

$$\delta_T \chi = -i \delta w(x) T \chi$$

and:

$$\delta_T L = -\frac{i}{2} \chi A^\mu T \chi \partial_\mu \delta w$$

i.e:

$$\delta_T L = j^\mu \partial_\mu \delta w$$

where $j^\mu = -\frac{1}{2} \chi A^\mu T \chi$ is a set of four hermitian op.

$$\text{and } \delta_T W_{12} = \int d\chi [j^\mu \partial_\mu \delta w] = \int d\chi [\partial_\mu \{ j^\mu \}_{T=0} \delta w(x)] - \delta w(x) \partial_\mu j^\mu$$

At this point the action principle tells us that $\partial_\mu j^\mu = 0$ as the 2nd term must vanish for arbitrary $\delta w(x)$. Therefore from such an invar prop. one obtains the above conservation law.

From the boundary term which comes from the volume integral of the divergence one obtains:

$$G = \int d\mu \int_T^\infty \delta w = T \delta w$$

where δw is const. at the boundary. T is the generator in Hilbert space of a unitary transf. which is induced by the transf T in the space of the field variables χ . In a suitable coordinate system:

$$T = \int d\mu j^\mu$$

Corresponding to the differential conservation law this quantity remains constant in time.

We can now infer the comm. rules. In general:

$$[\chi, G] = i \delta \chi = i [-i \delta w T \chi]$$

$$\text{Therefore: } [\chi, T \delta w] = \delta w T \chi$$

$$\therefore [\chi, T] = T \chi$$

Thus the commutator of the field with the operator T is determined by the finite dimensional matrix T . This establishes a correspondence between the infinit. transf. T acting in the finite dimensional space of internal degrees of freedom and transf. T' which represent a physical operator induced by T .

The most familiar example of such a physical quantity, expressed by the conservation of a current vector, is the electric charge. In analogy with this we come to a generalized notion of a charge as being the quantity whose conservation is a consequence of the invariance of the Lagrangian with respect to transf generated by the matrix T .

The more familiar non-hermitian fields which describe charge may be obtained by bringng T into diagonal form. Let

$$T \chi_{T'} = T' \chi_{T'}$$

where T' is some eigenvalue of T . Since T is imaginary one obtains

$$T \chi_{T'}^+ = -T' \chi_{T'}^+$$

and hence $\chi_{T'}^+ = \chi_{-T'}$

χ_T and χ_T^+ correspond to opposite signs of the eigenvalues of T , i.e. to opposite charges.

χ_T is a linear comb. of the variables X and hence from the comm. rel. for X one infers:

$$[\chi_T, T] = T' \chi_T,$$

By writing out the comm. rel. explicitly and allowing it to act on a state of definite eigenvalue T' of T one obtains:

$$T \chi_T |T'\rangle = (T' - T) \chi_T |T'\rangle$$

Thus the action of χ_T on a state vector $|T'\rangle$ is to decrease T' by an amount T , i.e. χ_T acts as a T annihilator provided, of course, that T is positive. Similarly χ_T^+ creates T . These are the familiar charge creation and annihilation operators.

In the case above, the internal degrees of freedom were characterized by a one parameter continuous group of transf. Now consider the general case of a n parameter continuous group of transf. Let Λ denote such a general infinit. transf.

$$\Lambda = 1 + i \sum_a S_{Wa} T_a \quad a = 1, \dots, n$$

Certain cond. must be satisfied if the Λ op. are to form a group. If Λ_f is a finite op. which is built up from an infinit. transf. the group prop. is satisfied only if $\Lambda_f^{-1} \Lambda \Lambda_f$ is another infinit. transf. of the same type as Λ , i.e. if

$$\Lambda_f^{-1} \Lambda \Lambda_f = 1 + \sum_a S_{Wa} \Lambda_f^{-1} T_a \Lambda_f$$

then $\Lambda_f^{-1} T_a \Lambda_f$ must be a linear comb. of the T_a . The same requirement applied to an infinit. transf. leads to the result:

$$[T_a, T_b] = \sum_c t_{abc} T_c \quad a, b, c = 1, \dots, n \quad (11)$$

where t_{abc} represent an array of numbers which characterize the comm. rel. and determine the internal symm. which may

possibly be described by continuous groups. From the imaginary character of the T 's and the antisymm. of the comm. one obtains

$$-t_{abc}^* = t_{abc}$$

$$t_{abc} = -t_{bac}$$

These numbers are not entirely arbitrary as they are closely related to the group structure. Consider the n matrices T_a as forming a vector in a certain n -dim space. If the index b is kept fixed then t_{abc} may be considered as a matrix in the same n -dim space in which T_a is a vector. The comm. rel. may be written in a matrix vector notation:

$$[T, T_b] = t_b T \quad (12)$$

The matrices t_b constitute a kind of represent. of the matrices T_b and hence must be obey the comm. rule:

$$[t_a, t_b] = \sum_c t_{abc} t_c \quad (13)$$

Specifically, the relation (12) sets up a correspondence between T_b and t_b from which, by making use of elementary comm. prop., one obtains:

$$[T, T_a], T_b] = t_a t_b T$$

$$[[T, T_b], T_a] = t_a t_b T$$

$$\begin{aligned} \therefore [t_a, t_b] T &= [[T, T_a], T_b] - [[T, T_b], T_a] = [T, [T_a, T_b]] = \\ &= \sum_c t_{abc} [T, T_c] = \sum_c t_{abc} t_c T \end{aligned}$$

Thus one immediately obtains eq. (13).

To emphasize the importance of the group requirements for our study, we observe that to every finite dim. T_a there corresponds an operator T_a in the infinite dim. Hilbert space:

$$T_a \rightarrow T_a = \frac{i}{2} \int d\delta_p \chi A^p T_a \chi \quad (14)$$

T_a should obey the same comm. rel. as T_a . Thus:

$$[T_a, T_b] = \sum_c t_{abc} T_c$$

These rel can be verified directly by making use of the field comm. rel. and the rel. for the op. T_a .

We have pointed out that the structure constants take form a rep. of the op. T_b . If they are to be a true rep., in the sense that the T_b matrices must fulfill the other requirements of the T_b matrices, then take must be antisymm. in a and c and imaginary. So, here:

$$T^T = -T \quad \text{and} \quad T^* = -T$$

there follows:

$$t_{abc} = -t_{cba}$$

$$\text{and} \quad t^* = -t$$

From the requirement of antisymm. on a, b and a, c it follows that t_{abc} is completely antisymm. in a, b, c

$$t_{abc} = -t_{bac} = t_{cfa} = -t_{cba} \quad (15)$$

For the general case, a study of the group requirements shows that the int. symm. group can be factored into a completely commutative group and an essentially non-comm. group, with a structure characterized by the prop. that the matrices T_b constitute a T matrix rep. of dim. = n , the number of transf. parameters. Hence the main problem is the investigation of essentially non-comm. groups with a structure given by (15).

For $n=1$ or 2 t_{abc} is zero and the T 's commute. The 1st examples of the latter type are encountered for $n=3$ and $n=6$. For $n=3$ one can write:

$$t_{abc} = \epsilon_{abc} t_{123}$$

where $\epsilon_{abc} = 1$ for an even permutation of a, b, c and = -1 for an odd permutation. The factor t_{123} must be imaginary. As a scale factor is at our disposal we may take

$$t_{123} = i$$

and thus obtain:

$$[T_1, T_2] = i T_3 \quad [T_2, T_3] = i T_1 \quad [T_3, T_1] = i T_2 \quad (16)$$

The group structure is that of the 3-dim. Euclidian rotation group (the matrix Λ , of which T is the generator is orthogonal). Therefore only Euclidian groups occur. This is just the kind of classification that is empirically introduced with the notion of isotopic spin, a notion which is used to represent the observed prop. of the various multiplets of particles.

There is nothing essentially new for $n=4$ or 5 . These are obtained by adding one or two transf. rep., which commute with all the transf.

For $n=6$ something new can be obtained. To the matrices T_1, T_2, T_3 obeying the above comm. rules one can add a set Z_1, Z_2, Z_3 obeying similar rules such that every Z commutes with every T .

This is the only obvious possibility. This group can be presented in another way. It is equivalent to the group of Euclidian rot. in a space of 4 dim. From this aspect it is perfectly clear why must jump from $n=3$ to $n=6$. We are exploring the symm. prop. characterized by the rep. of the Euclidian rot. groups. The independent op. are rot. in the various orthogonal coordinate planes. For a V dim. space there are $\frac{1}{2} V(V-1) = n$ such planes. Thus

$$V = 2, 3, 4, \dots$$

$$n = 1, 3, 6, \dots$$

The infinit. generators T , of rot., are conveniently described by means of an anti-symm. tensor T_{abc} satisfying the comm. rel.

$$\frac{1}{i} [T_{ab} T_{cd}] = S_{ac} T_{bd} - S_{bc} T_{ad} + S_{ba} T_{dc} - S_{ad} T_{bc} \quad (17)$$

On coming back to the 3-dim group, a comparison of notation yields:

$$T_{23} = T_1 \quad T_{12} = T_3 \quad T_{32} = T_2$$

For $v=4$ there are six such generators T_{ab} . One can easily verify that they may be grouped in two sets of three as follows:

$$T_3 = \frac{1}{2} (T_{12} + T_{34}) \quad \text{and cyclic permutations of } 1, 2, 3 \\ Z_3 = \frac{1}{2} (T_{12} - T_{34}) \quad \text{and cyclic perm. of } 1, 2, 3. \quad (18)$$

From the comm. rel. for T_{ab} there follows the comm. rel. mentioned above for the T 's and Z 's. Thus the four dim. rot. group can be split into two indep. factors, each of which has the prop. of the three dim. rot. group. This is as far as we shall need to go in order to get something of interest for Physics.

We have been examining the possibilities of int. structure by considering larger and larger numbers of indep. trans. As a kind of complementary investigation one can ask, what are the kinds of symm. that can be represented by the operation of matrices upon field quantities of higher and higher multiplicity? If we have a very small multiplicity, we can expect to represent only a very small number of int. symm. prop. The next step is to examine what happens as the multiplicity increases.

Let us consider transf. in a v -dim space, i.e. we consider operations upon the field χ with components in the internal space. The T matrices which operate on χ must be anti-symm. and the number of indep. op. that one can perform is simply the number of linearly indep. anti-symm. matrices which one can construct. There are $\frac{1}{2}v(v-1)$ such matrices. The elementary indep. antisymm. matrices are of the form:

$$\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ 0 & i & 0 \end{pmatrix} \quad \text{etc.}$$

where each matrix possesses v rows and columns. The totality of these gives us a set possessing the required number of matrices. Each matrix generates a rotation in one of the coordinate planes

of the v dim. vector space.

The elementary matrices can be represented in analytic form as follows:

$$(T_{ab})_{cd} = \frac{1}{i} (\delta_{ac} \delta_{bd} - \delta_{ad} \delta_{bc})$$

The indices a, b define the particular matrix. The indices c, d define the row and columns. One can verify that the proper comm. rel. are satisfied.

In this way one obtains simple rep. of the rot. groups in the corres. spaces of appropriate dimensions. These are characterized among other things by the characteristic values of these matrices. The eigenvalues of T_{ab} are:

$$T_{ab} = 0, \pm 1$$

The eigenvalue 0 corresponds to a vector which is not in the plane (a, b) . The eigenvalue ± 1 correspond to the sense of the rotation. Zero will always occur as an eigenvalue with the exception of the 2 dim. case.

For $v=2$ there is just one anti-symm. matrix

$$T_{12} \sim \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

This corresponds to a physical prop. like electric charge whose eigenvalues are ± 1 .

For $v=3$ there are three anti-symm. matrices:

$$\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

The characteristic values are 0, ± 1 . We call these $T=1$ (corresp. to ang. mom. 1). In particular we do not find the rep. which corresponds to the quantum number $\frac{1}{2}$. Mathematically, this is the rep. from which everything else can be constructed. Since there is good evidence that the internal prop. of neutrons and protons can be described by this number we must at least go on to $v=4$.

For $D=4$ there are 6 antisymm. matrices which can be interpreted as the transf. of a vector quantity having 4 comp. If one looks at this space from the stand point of 3+1 dim. one obtains the $T=1$ (vector) and $T=0$ (scalar) rep. of the 3-dim group. Alternatively eq. (18) can be used to represent a 4-dim rot as a direct product of two 3-dim rot. From the given forms of Tab. one easily obtains the result that the characteristic values of T_3 are $\pm \frac{1}{2}$. A similar result holds for Z_3 and thus one obtains the $T=\frac{1}{2}$ rep. twice over.

In this way, the 6 fundamental rot. matrices can be regarded in terms of 3-dim either as $T=1$ and $T=0$ or as $T=\frac{1}{2}$ twice over. Since the fundamental $T=\frac{1}{2}$ rep. of the 3-dim rot. group, familiar as isotopic spin, is first encountered within the framework of 4-dim symm., it is natural to suppose that the latter is the fundamental underlying symm. and that fields exist which realize the two-fold $T=\frac{1}{2}$ rep. and the equivalent $T=0, 1$ representation. The distinction between integral and half-int T only appears when the 4-dim symm. are reduced to 3-dim ones.

The reduction to 3-dim symm. should distinguish physically the two $T=\frac{1}{2}$ reps. as well as the $T=0$ and $T=1$ rep. Now we know in fact that, these 3-dim symm. are only approx., that the E.M. field is the physical agency that destroys the 3-dim isotopic space symm. and leaves only a 2-dim symm. This field, physically distinguishes the various members of these isotopic spin multiplets and one naturally infers that it is the agency which gives rise to mass differences among the members.

In the 3-dim isotopic space the EM field will distinguish one plane among the three. This is taken to be the 1-2 plane. In this case we have the great advantage of knowing the physical agency that breaks down the 3-dim

symm. and we know that the two-dim symm. which is left implies the conservation of the associated physical quantity, electrical charge. Now we can identify the four 3-dim reps. by means of the 2-dim rep. into which they finally degenerate.

In accordance with the distinguishability of the 1-2 plane, T_{12} is identified with electrical charge Q . In terms of the 3-dim rep., Q will appear in different ways according to the mode taken in the breakdown from 4 to 3 dim, e.g. We can simply narrow our sights from four axes to three by picking out

$$T_1 = T_{23}, \quad T_2 = T_{31}, \quad T_3 = T_{12}$$

This is the reduction giving the characteristic values $0, \pm 1$, the $T=1$ rep. Then there is a second possibility:

$$T_3 = \frac{1}{2}(T_{12} + T_{34})$$

$$Z_3 = \frac{1}{2}(T_{12} - T_{34})$$

from which

$$T_{12} = T_3 + Z_3$$

This gives the $T=\frac{1}{2}$ rep.

These reductions can be combined in the following way like T_3, Z_3 has eigenvalues of $\pm \frac{1}{2}$. Hence one may set

$$Q = T_{12} = T_3 + \frac{1}{2}Y$$

where $Y=0$ if T integral and $\pm \frac{1}{2}$ if $T=\frac{1}{2}$. Y is a new quantity which is defined in order to unify the two different ways of looking at the underlying 4-dim structure. It can be shown that this new quantity can be defined in terms of an invariance with respect to a rotation. The quantity Y is called hypercharge. It takes the values $0, \pm 1$ and classifies the hyperons. Thus, from the geometrical interpretation of the 4-dim structure, the two 3-dim realizations, the way in which they are related finely to the common 2-dim rot. that has a specific identification of electrical charge, how all this, one has a

recognition of the charge monopoles that will be associated with the various mathematical constructions.

Invariancia Relativista y Representaciones proyectivas del Grupo de Lorentz

(A.S. Wightman en les Problèmes Math. de la Théorie Quantique des Cléamps. Lille 1957. Cf. también: E.P. Wigner. Ann. of Math. 40, 149, 1939. V. Bargmann et E.P. Wigner Proc. Nat. Acad. Sci., 34, 211, 1946, E.P. Wigner, N. Cimento 3, 517, 1956)

En la T. de la Rel. especial, cada observador equivalente (cuyo número es infinito) emplea cuatro coord. para describir su posición en el espacio tiempo. Sean estas $x^i = ct$ ($c = \text{vel de la lsg}$ y $t = \text{tiempo}$) y x^i con $i=1,2,3$. Cada una de estas descripciones está relacionada con las otras a través de las transf. inhomogéneas de Lorentz:

$$\begin{aligned} y &= \Lambda x + a \\ y^i &= \Lambda^{ij} x^j + a^i \end{aligned} \quad \left. \right\} (1)$$

donde a es una transloción en el esp. y en el tiempo y Λ es una transf. inhomogénea de Lorentz, esto es, por def. es una matriz 4×4 tal que:

$$(\Lambda x) \cdot (\Lambda y) = x \cdot y \quad (2)$$

para todos cuadivectores reales x y y . Aquí:

$$x \cdot y \equiv x^0 y^0 - x^i y^i$$

Las transf. homog. de Lorentz forman un grupo multiplicativo, el grupo homog. de Lorentz. Este grupo está formado por cuatro partes conexas caracterizadas por los signos de $\det \Lambda$ y de Λ^0 . Llamaremos grupo resringido al subgrupo conexo definido por $\det \Lambda = 1$ y $\Lambda^0 > 0$. Esta terminología es inmediatamente aplicable

al grupo de Lorentz entero, cuyos elementos escribiremos como $\{a, \Lambda\}$. Por ej. el grupo entero se compone de 4 partes conexas cuyos elementos $\{a, \Lambda\}$ representan una translación arbitraria a en el esp. tiempo y Λ es una de las cuatro partes del G. homog. ya mencionadas.

El cubiniento universal del G. Lorentz resringido homog. consta de dos hojas y es isomorfo al grupo de todas las matrices complejas 2×2 con determinante 1, llamadas grupo unimodular. La relación entre los dos grupos puede expresarse como sigue: para cada cuadivector real X , podemos escribir una matriz hermitiana 2×2 , \bar{X} :

$$\bar{X} = x^0 \cdot 1 + \sigma^i X^i \quad (3)$$

$$\text{donde } 1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \left. \right\} (4)$$

$$\sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Recíprocamente todo matriz hermitiana 2×2 , \bar{X} determina un cuadivector real que satisface (3). Una matriz compleja A (2×2 con $\det A = 1$) determina una transf. lineal:

$$\bar{X} \rightarrow \bar{X}' \quad \text{donde } \bar{X}' = A \bar{X} A^* \quad (5)$$

Esta transf. lin. es una transf. resringida de Lorentz, con la cual puede obtenerse cualquier otra. Evidentemente $\pm A$ corresponde a la misma transf. de Lorentz. En general es más fácil trabajar con el G. unimodular entero, el cual escribiremos $\{a, \Lambda\}$ (Λ es un elemento del G. unimodular) y cuya ley de multiplicación es:

$$\{a_1, \Lambda_1\} \cdot \{a_2, \Lambda_2\} = \{a_1 + \Lambda_1 a_2, \Lambda_1 \Lambda_2\}$$

donde Λ_1 es la transf. homogénea de Lorentz determinada por Λ_1 .

Escribiremos $\{a, \Lambda\}$ en vez de $\{a, A\}$ simplemente por "abuso de lenguaje".

La Mec. Cuántica describe los estados puros de un sist. fís. mediante vectores unitarios en un esp. de Hilbert. Proviamente hablando no se trata de vectores unitarios que no son de

clase de equivalencia definida por todos los vectores unitarios que no difieren más que por una constante multiplicativa de módulo 1. Para una teoría cuántica, relativisticamente invariantes, existe, para todos los vectores Φ y toda transf. de Lorentz infinitesimal $\{a, \Lambda\}$, un vector $\Phi(a, \Lambda)$ que satisface la condición:

$$|\langle \Phi, \Phi \rangle|^2 = |\langle \Phi(a, \Lambda), \Phi(a, \Lambda) \rangle|^2 \quad (7)$$

(Hipótesis de invariancia rel.). Esta condición puede sólo afirmarse para vectores Φ y Ψ que describen estados realmente realizables en el laboratorio y se sabe bien que no todos los vectores representan uno de tales estados. Nuestra experiencia hasta el presente ~~nos~~^{no} nos da todo suficiente conocimiento sobre la estructura de esos estados físicamente realizables y para poder seguir nuestro análisis es necesario hacer una hipótesis un poco arbitraria: el espacio de Hilbert H_i es la suma directa de subespacios H_i tales que a todo vector de H_i corresponde un estado físico observable y todo estado puro, físicamente observable, está representado por un vector perteneciente a uno de esos H_i . (Esta hipótesis es equivalente a suponer que el anillo de operadores que comunitan con todos los observables es comunitativo, incluyendo que, más generalmente, $\sum H_i$ puede ser una integral directa en vez de una suma directa). Se dice que todo operador que comunica con todos los observables define una regla de superselección. Cf. G. Wick, A.S. Wightman y E.P. Wigner Phys. Rev. 88, 109, (1952). Si se supone verificada esta hipótesis y (7) es válida en cada H_i , se puede demostrar que para una selección conveniente de vectores Φ y $\Phi(a, \Lambda)$, se puede definir un operador $U(a, \Lambda)$ tal que $\Phi(a, \Lambda) = U(a, \Lambda) \Phi$ donde $U(a, \Lambda)$ es unitario o antiunitario. Un operador U es antiunitario si esto define para todos los vectores y satisface: $U(\alpha \Phi) = \alpha^* U \Phi$, $U(\Phi_1 + \Phi_2) = U(\Phi_1) + U(\Phi_2)$

$$\text{y: } (\Phi_1, \Phi_2)^* = (U \Phi_1, U \Phi_2)$$

para todos los vectores Φ, Φ_1, Φ_2 y escalar α). Mas aún, se encuentra que en cada uno de los subespacios H_i , $U(a, \Lambda)$ está determinado de manera única hasta una constante multiplicativa. De acuerdo con la ley de mult. de las transf. de Lorentz, los estados descritos por los vectores $\Phi(a_1, \Lambda_1) \cdot (a_2, \Lambda_2)$ y $\Phi(a_1 + \Lambda_1 a_2, \Lambda_1 \Lambda_2)$ son idénticos. Esto implica que los operadores $U(a_1, \Lambda_1) U(a_2, \Lambda_2)$ y $U(a_1 + \Lambda_1 a_2, \Lambda_1 \Lambda_2)$ difieren solamente en un factor multiplicativo de módulo 1 en cada subespacio H_i :

$$U(a_1, \Lambda_1) U(a_2, \Lambda_2) = w(a_1, \Lambda_1; a_2, \Lambda_2) U(a_1 + \Lambda_1 a_2, \Lambda_1 \Lambda_2) \quad (8)$$

Obviamente se podrá ver diferente en subespacios diferentes H_i de tal manera que debe ser considerado de hecho, como el operador $\sum w_i E_i$ donde $|w_i| = 1$ y E_i es el operador de proyección sobre H_i .

El cuadrado de un operador antiunitario es unitario. Resulta que $U(a, \Lambda)$ es unitario cuando $\{a, \Lambda\}$ pertenece al grupo restringido, ya que cada elemento de este grupo puede escribirse como producto de elementos que son cuadrados. Para determinar si $U(a, \Lambda)$ debe ser unitario o antiunitario para las otras tres partes conexas del grupo, será suficiente examinar $U(0, is)$ y $U(0, it)$ donde:

$$(isX)^0 = X^0 \quad (isX)^j = -X^j \\ (itX)^0 = -X^0 \quad (itX)^j = X^j \quad (j = 1, 2, 3)$$

ya que todos los demás elementos de las otras partes pueden escribirse como el producto de un elemento del grupo restringido y de is^0 ó it^0 ó $isit$.

Encontraremos posteriormente, por razones físicas, que $U(0, is)$ debe ser unitario y $U(0, it)$ antiunitario. El operador $U(a, \Lambda)$ puede ser reemplazado por $e^{i\alpha(a, \Lambda)} U(a, \Lambda)$, con α real sin cambio en nada la correspondencia entre vectores $\Phi \rightarrow \Phi(a, \Lambda)$. Se puede entonces hacer una selección particular de $\alpha(a, \Lambda)$ para facilitar el tratamiento matemático. En particular, se hace la hipótesis física de la continuidad de la expresión $|\langle \Phi, \Phi(a, \Lambda) \rangle|$ respecto a $\{a, \Lambda\}$ y que de mostar que $U(a, \Lambda)$ y w pueden ser tomadas como continuas respecto a los productos del grupo (Cf. E.P. Wigner, Ann. of Math. 40, 149, 1939).

Así, en toda teoría cuántica invarianta relativista, que satisface la hipótesis anterior para las reglas de superselección, hay una representación continua del grupo de Lorentz inhomogéneo, dividida hasta un factor, seguramente. Para distinguir al comportamiento posible de una teoría cuántica relativista frente a las transf. inhomogéneas de Lorentz, es suficiente clasificar las representaciones continuas del grupo inhomogéneo de Lorentz excepto por un factor.

La teoría de la clasificación emplea por normalizar el factor w_i . Se puede demostrar que, para el grupo resstringido, el factor de fase $e^{i\lambda}$ puede seleccionarse siempre de tal manera que el factor w_i sea ± 1 y de manera que la representación continua del grupo sea, hasta un factor, una representación continua del grupo de recubrimiento. Se sabe, de acuerdo con la teoría clásica de la representación del grupo de translaciones que:

$$U(a, t) = e^{i P^{\mu} a_{\mu}}$$

donde P^{μ} ($\mu = 0, 1, 2, 3$) son operadores antisimétricos que representan físicamente la energía y el momento. De la ley de multiplicación del grupo resulta que el aspecto de los P^{μ} es invariante frente a las transf. del grupo resstringido de Lorentz. Si se impone entonces la condición física de que existe una constante anterior a la energía, la ley de mult. del grupo obliga a tener $U(0, is)$ unitaria y $U(0, it)$ antunitaria.)

Se puede mostrar que toda representación continua del grupo unimodular inhomogéneo es una integral directa de representaciones irreducibles y que las representaciones irreducibles son unitariamente equivalentes, si, y solamente si: 1) las medidas que son integrales directas difieren por equivalentes y 2) las multiplicidades con las cuales las representaciones irreducibles aparecen son iguales casi donde quiera respecto de la medida ν_{μ} . (Cf. G. W. Mackey. Proc. Acad. Sci. 35, 537 (1949); Ann. of Math. 58, 193, (1953)). Cada representación irreducible del grupo resstringido tiene un valor bien definido de $P_{\mu} P^{\mu} = m^2$ siendo el numero

real no negativo ni la masa del sistema. Para $m \neq 0$ las representaciones irreducibles están numeradas por el spin j que toma los valores $0, \frac{1}{2}, 1, \frac{3}{2}, \dots$, j está definido por la relación:

$$W = -m^2 j(j+1) \quad (9)$$

donde $W = w^{\mu} w_{\mu}$ y $w^{\mu} = \frac{1}{2} \epsilon^{\mu \lambda \kappa \nu} P_{\lambda} M_{\kappa \nu}$ y $M_{\mu \nu}$ es la transf. infinit. de Lorentz del plano $\mu\nu$. Para $m=0$, hay dos clases de representaciones: aquellas con $W \neq 0$ que no tienen, aparentemente, significado físico y aquellas con $W=0$. Ignoraremos la primera clase. La segunda está numerada por un spin $\pm j$ con $j = 0, \frac{1}{2}, 1, \dots$, que satisface:

$$w^{\mu} = \pm j P^{\mu} \quad (10)$$

Cuando se pasa del grupo resstringido al grupo que contiene las simetrías, se encuentra que la masa y el spin continúan numerando las representaciones irreducibles hasta un factor, pero que para $m \neq 0$, hay, para cada masa y spin, cuatro repr. irreducibles correspondientes a los cuatro posibilidades $U(0, it)^2 = \pm 1, U(0, is)^2 = \pm 1$. En el caso $m=0$, las representaciones "izquierdas" y "derechas" corresponden a los signos \pm en (10) muy claramente, pero todavía hay cuatro repr. más, hasta un factor, irreducibles para cada j , correspondientes a las cuatro posibilidades mencionadas anteriormente.

Naturalmente el grupo de Lorentz inhomogéneo posee otras repr. irreducibles que las cuales el aspecto del momento contiene momentos espaciotemporales, o no contiene mas que el punto $p=0$ y no es sencillo que estas representaciones intervengan en la teoría cuántica relativista, por ej. en las prop. de transf. de los campos. Estas repr. han sido clasificadas por V. Bargmann: Ann. of Math. 48, 568 (1947) y I. Gel'fand y M. Naumov, Bull. Acad. Sci. URSS Ser. Mat. II, 411 (1947). Pero vale la pena subrayar que, en las prop. de transf. de estados, solo pueden intervenir las repr. numeradas anteriormente y la repr. por la identidad, que describe el vacío. Esto basta, al cual se refiere uno frecuentemente por lo poco q "no hay estados de energía negativa", es de importancia capital en el análisis de los campos y de los valores

medios en el vacío.

La sola invariancia de Lorentz sólo conduce a dos reglas de superselección: una de univocidad según la cual los estados que se transforman de acuerdo con representaciones univalentes del grupo de Lorentz son homogéneos rotando, no son superponibles a estados que se transforman siguiendo representaciones bivalentes. En términos más físicos, esto quiere decir que los estados de spin semienteros no son superponibles a los de spin enteros. Esta regla de selección es válida, independientemente de que la teoría sea, o no, invariantes respecto a las simetrías. La otra regla de superselección es una regla de diferentes tipos, según la cual los estados para los cuales una operadora de simetría antimaterial con cuadradito +1 no es superponible a aquellos cuyo cuadradito es -1 y esta regla no es válida más que en una teoría invariantes por simetría.

Resumamos los resultados de este análisis general de invariancia relativista. Una teoría cuántica relativista está encuadrada en un espacio de Hilbert \mathcal{H} que es una suma directa de espacios de Hilbert \mathcal{H}_i . Las reglas de superselección de la teoría afirman que todo estado puro está descrito por un vector perteneciente a uno solo de los espacios \mathcal{H}_i y que, reciprocamente, cada vector de un \mathcal{H}_i describe un estado. Existe en \mathcal{H} una representación continua del grupo unimodular inhomogéneo que está determinada, hasta una equivalencia unitaria, por una medida positiva sobre la parte no negativa del eje real, que define el espectro de masas, y por las funciones de multiplicidad que indican cuantas veces las representaciones de cada spin intervienen para cada masa. (Si la teoría es invariantes por simetrías, se debe también distinguir, para cada masa y spin, los diversos tipos) La representación por la identidad, proveniente del estado de vacío, debe ser considerada por separado.

Existen otras consideraciones como las principales transformaciones

A Simple Derivation of Meson Scattering. V. F. Weisskopf

I. Phase shift and Boundary Conditions.

We assume that the interaction between a meson and a nucleon acts only at short range $r_0 \ll 1$. (Units of length is (\hbar/mc) where m is meson mass). We assume the nucleon fixed in space. Static meson theory. The meson is free particle for $r > r_0$. (r is distance between meson and nucleon). We assume that only p-waves interact.

The interaction determines the logarithmic derivative for $r = r_0$ which we call f :

$$f = r_0 \left(\frac{u'(r)}{u(r)} \right)_{r=r_0}$$

where $u(r)$ is r times the wave function of the meson;
 $u(r)$ is given by ($z = kr$, δ is the phase shift)

$$u(r) = \cos \delta \left(\cos z - \frac{\sin z}{z} \right) - \sin \delta \left(\sin z + \frac{\cos z}{z} \right) \xrightarrow[r \rightarrow \infty]{} \cos(z + \delta)$$

and we can calculate the phase shift in terms of f , expanded in powers of k^2 .

$$(1) \quad k^3 \cot \delta = \frac{3}{r_0^3} \left(\frac{f+1}{2-f} - G(f) k^2 r_0^2 + \dots \right), \quad G = \frac{3}{5} \frac{f^2 - 3f + 1}{(2-f)^2}.$$

f is a slowly varying function of the energy, since it is determined in a small volume $r < r_0$, where the characteristic energies are high. We therefore expand f , or rather g

$$q = \frac{k+1}{2-f}$$

(2)

in terms of the energy $\omega = \sqrt{k^2 + 1}$:

$$(2) q = q_0 + q_1 \omega + q_2 \omega^2$$

We then get

$$(3) k^3 \cot \delta = \frac{3}{k_0^3} (q_0 + q_1 \omega + (q_2 - C k_0^2) \omega^2 + C k_0^2 + \dots)$$

$$C = \frac{1}{3} \frac{1 - q - q^2/5}{1+q} \sim \frac{1}{3} \frac{1 - q_0 - q_0^2/5}{1+q_0}$$

Since k_0 is very small, it is allowed to replace q by q_0 in the expression for C .

Since there are four different meson-p-waves, (corresponding to the well-known 33, 31, 13, 11 spin combinations) we have actually four equations of the form (3).

The scattering would be determined if we knew the magnitudes q_0, q_1, q_2 for the four states. We will show that an investigation of the meson field of a nucleon at almost static conditions gives us all the information, namely:

$$(4) q_0 \approx 0 \text{ for all four states}$$

$$q_1 \approx -\frac{\mu_0^3}{g^2 \lambda_i} \text{ where } g^2 \text{ is the coupling constant and } \lambda_i = (+4, -2, -2, -2)$$

$q_2 \ll C k_0^2$ and therefore negligible.

* actually the strength constant of nuclear-meson force at large distance.

II. The Static Meson field and Meson scattering at energies below Rest mass.

(3)

Consider a nucleon 1 and its static meson field at the distance \vec{r} ; where $|r| \gg 1$:

$$(5) \phi_1 = g T_1(\vec{O}, \vec{n}) \frac{e^{-kr}}{r}$$

Here g is the renormalized coupling constant which, per definition, determines the meson field at large distances; \vec{n} is the unit vector parallel to \vec{r} .

We now put a second nucleon 2 at a large distance R from the nucleon 1. We arrange it such that it exchanges its spin (orbital mechanical or isotopic) with 1 in such a way that its meson field ϕ_2 is periodic in time. The distance R is chosen so great that the exchange takes place extremely slow, so that ω^2 terms can be neglected. Under these conditions the space dependence of the meson fields is not different from the static one since the wave number $k = (\omega^2 - 1)^{1/2}$ and therefore deviates from the static value $k = i$ only by terms of order ω^2 .

We then expect, that also the meson field ϕ_1 of the first meson has a periodic part. The whole set-up is then a scattering set up, with the field $\phi_2(0)$ at $r=0$ (the pole of 1)

as the incident field ϕ_{inc} and the periodic part of ϕ_i , being the scattered field ϕ_{sc} . We can define the scattering amplitude γ by:

$$(6) \quad \gamma = \phi_{\text{sc}} = \phi_{\text{inc}} \gamma \frac{e^{+ikr}}{r} = \phi_{\text{inc}} \gamma \frac{e^{-r}}{r}$$

The scattered field we get as follows*: The Hamiltonian of the nucleon I under the influence of the second one is given by

$$(7) \quad H = g(\vec{\sigma}_1 \nabla)(T_1 \phi_2(0)) - g(\vec{\sigma}_1 \vec{n}_0)(T_1 \phi_2(0))$$

where \vec{n}_0 is the unit vector in the direction up towards the second nucleon, and neglecting terms $\sim R^{-2}$. We now get the periodic part of the field ϕ_i (by calculating its time derivative and dividing it by $i\omega$):

$$(8) \quad \dot{\phi}_{\text{sc}} = \frac{1}{i\omega} [H, \phi_i] = -\frac{g^2}{\omega} [(\vec{\sigma}_1 \vec{n}_0) T_1^{(0)}, (\vec{\sigma}_1 \vec{n}) T_1^{(1)}] \phi_2(0) \frac{e^{-r}}{r}$$

Here $[\alpha, \beta]$ is the commutator of α and β ; $T_1^{(0)}$ and $T_1^{(1)}$ are the components of the isotropic spin of I in the direction of the incident field and in the direction of the scattered field. Note that $\phi_2(0)$ commutes with H .

The commutator in (8) is a well-known quantity which is

* The following consideration is due to Julian Schwinger.

diagonal in the four spin states. We have

$$[(\vec{\sigma}_1 \vec{n}_0) T_1^{(0)}, (\vec{\sigma}_1 \vec{n}) T_1^{(1)}] = \lambda_i, \quad \lambda_i = \begin{pmatrix} 4 & & & \\ -2 & -2 & & \\ & & -2 & \\ & & & -2 \end{pmatrix}.$$

Comparing (8) with (6) we get immediately

$$(9) \quad \gamma_i = -\frac{g^2}{\omega} \lambda_i$$

which shows the fact that the scattering amplitude has a pole at $\omega=0$.

It is now easy to express the information contained in (9) in terms of the cot δ , in order to compare it with (3). We use the well-known formula connecting γ with cot δ for p-waves:

$$\gamma = k(\cot\delta - i) = \frac{3}{2}$$

If ω is very small, we can put $k=i$ and we write, if ω^2 -terms are neglected:

$$k^3 \cot\delta = -\frac{3}{2} + i$$

Putting in the value (9) we get

$$(10) \quad k^3 \cot\delta = 1 + \frac{3}{g^2 \lambda_i} \omega + (\text{terms in } \omega^2)$$

Now we compare this with (3) and see immediately

$$(11) \quad q_0 + C r_0^2 = \frac{r_0^3}{3}, \quad q_i = -\frac{r_0^3}{g^2 \lambda_i}$$

Because of the smallness of r_0 , the first equation is equivalent to

$$(12) \quad q_0 \approx 0 \quad \text{and from (3): } C \approx \frac{1}{3}.$$

This means that $f = -1$ for $\omega = 0$.

We have not yet determined q_2 . We will show that it can be neglected compared to $C_{r_0}^2$. From the expansion (2) we expect the order of magnitude of q_2 to be $q_2 \sim q_1^2$, and hence $q_2 \sim r_0^6 / (g^4 \lambda_i^2)$. It is easier to estimate q_2 if we determine the magnitude of q_1 from the position of the resonance in the 33 state. If q_2 is negligible compared to $C_{r_0}^2$, we see from (3) (and (12)) that the resonance frequency ω_{res} is ($\cot \delta = 0$)

$$(13) \quad \omega_{\text{res}} \approx \frac{3q_1}{r_0^2}$$

and hence $q_1 \approx \frac{1}{3} \omega_{\text{res}} r_0^2 \approx (q_2)^{1/2}$.

Comparing now q_2 with $C_{r_0}^2$ we obtain:

$$(14) \quad \frac{q_2}{C_{r_0}^2} \approx \frac{3q_1^2}{r_0^2} \approx \frac{1}{3} (\omega_{\text{res}} r_0)^2.$$

This ratio is reasonably small as long as ω_{res} is smaller than the "cut-off" frequency ω_0^{-1} . In fact, we can find a

from (11) and (13):

$$r_0 = \frac{1}{3} g^2 \lambda_{33} \omega_{\text{res}}.$$

With the observed value $\omega_{\text{res}} \approx 2$ and $g^2 \approx \frac{1}{10}$, we get $r_0 \approx \frac{1}{4}$. The ratio (14) is therefore about $\frac{1}{12}$ and our results in (4) are reasonably justified.

We now can write (3) in the following form, neglecting q_2 :

$$\boxed{\frac{k^3}{\omega} \cot \delta_i - \frac{1}{\omega} = \frac{3}{g^2 \lambda_i} - \frac{\omega}{r_0}}$$

This is the effective range approximation formula for the scattering phase shift. It differs from the Chew-Low result by the "Serber term" $\frac{1}{\omega}$. The first term on the right is determined by the "scattering" near $\omega = 0$, i.e. the static meson field at large distances; the second term on the right does not depend on the spin state. It is, in this approximation, solely depending on the fact that there is only p-wave interaction.

Causality Conditions.

We want to enquire into the existence of general conditions on the scattering phase shifts. Such conditions or restrictions do exist, owing to the wave-nature of the scattering, and are described under the general heading of "causality" conditions. These arise, essentially, from the requirement of special relativity that no signal can be transmitted with speed greater than that of light. They are based on the observation that the propagation of a wave through a medium is determined by the scattering properties of the elementary scatterers in the medium - in particular, by the forward scattering and absorption. That there is an intimate connection between forward scattering and absorption.

a) Wigner's weak causality conditions:

A very simple limitation on the possible scattering phase shifts, arising from causality requirements, has been pointed out by Wigner (E.P. Wigner. Phys Rev. 98, 145, 1955). The origin of this condition can be seen if we consider, as the simplest example, a spherical wave packet impinging on a scattering center. The wave packet is made up of a superposition of components of wave number k and frequency ω (for a particle wave, $k = P/h$, $\omega = E/h$, $v_p = \omega/k$ = phase velocity) each of which has the form:

$$\psi_i = \frac{1}{r} e^{-i(kr+wt)} \quad (1)$$

For extreme simplicity, we will make a wave packet out of just two frequencies, centered about ω ,

$$\psi_i = \frac{1}{r} [e^{-i(k+\delta k)r} - i(w+\delta\omega)t + e^{-i(k-\delta k)r} - i(w-\delta\omega)t] \quad (2)$$

The center of this packet (defined as the space-time point at which the two phases are equal) moves with the group velocity

$$v = -\frac{\delta\omega}{\delta k} \quad (3)$$

Now, let the phase shift of the scattered wave to be $\alpha(\omega)$; then this has the asymptotic form

$$\psi_o = \frac{1}{r} [e^{i(k+\delta k)r} - i(w+\delta\omega)t + 2i(\alpha+\delta\alpha) + e^{i(k-\delta k)r} - i(w-\delta\omega)t + 2i(\alpha-\delta\alpha)] \quad (4)$$

The center of the scattered outgoing packet is, by the same

criterion as mentioned above:

$$(\delta k)r - (\delta\omega)t + 2(\delta\alpha) = 0$$

$$\therefore r = \frac{\delta\omega}{\delta k}t - 2\frac{\delta\alpha}{\delta k} = vt - 2\frac{d\alpha}{dk} \quad (5)$$

Thus the scattered wave is retarded in time (with respect to the situation for zero phase-shift) by an amount

$$\Delta t = -\frac{2}{v}\frac{d\alpha}{dk}$$

note that for $\frac{d\alpha}{dk} < 0$, the wave is advanced in time.

The causality condition comes from the observation that, provided the scatterer has a finite range R , the maximum advancement of the wave packet consistent with the relativity postulate is:

$$\Delta t_{\max} = \frac{2R}{v}$$

since the scattered wave cannot appear before the incident wave reaches the finite boundary of the scattering center. Thus,

$$\frac{2R}{v} \geq -\frac{2}{v}\frac{d\alpha}{dk}$$

$$\text{or: } \frac{d\alpha}{dk} \geq -R \quad (6)$$

It is to be noted that equation (6) implies a limitation only for phase shifts with negative derivatives, since only such scattering implies an advancement in time for the scattered wave. There is no limitation on the degree to which a center can retard the emission of the scattered wave.

The above derivation has been oversimplified in that the incident wave was taken as spherical. For a plane incident wave, a partial wave analysis, together with the scattering formalism of Wigner and Eisenbud, permits a causality limitation to be established on the phase shifts corresponding to each angular momentum component of the wave. These have been shown by Wigner to be, for s and p waves:

$$\left. \begin{aligned} \frac{d\alpha_0}{dk} &\geq -R + \frac{\sin 2(\alpha_0 + kR)}{2k} \\ \frac{d\alpha_1}{dk} &\geq -R + \frac{1 - \cos 2(\alpha_1 + kR)}{k^2 R} - \frac{\sin 2(\alpha_1 + kR)}{2k} \end{aligned} \right\} \quad (7)$$

As a first application of the weak causality conditions, we consider the requirement on the low energy behavior of the phase shifts. Let $\alpha \rightarrow -ak^n$, with $n \geq 1$. Then, for s-waves

we have the condition:

$$n a_0 k^{n-1} \leq a_0 k^{n-1}$$

or $n=1$, while for p waves:

$$n a_1 k^{n-1} \leq 3 a_1 k^{n-1} - \frac{2}{R} (a_1 k^{n-1})^2$$

or $n \leq 3$. These conditions are, of course somewhat weaker versions of the general quantum mechanical conditions derived on the low energy phase shifts for scattering by a finite potential.

b) Strong causality conditions. — The dispersion relationship of Kramers and Kronig.

In optics, there has long been recognized a connection between the amplitude for forward scattering of electromagnetic waves and the absorption cross section of the elementary oscillators responsible for the scattering. This connection known as the dispersion relation ship, was first derived by Kronig (R. de L. Kronig. J. Opt. Soc. Am. 12, 547, 1926) and by Kramers (H.A. Kramers, Congr. Inter. Fisici Como 2, 545, 1927) on the basis of the electron oscillator model of optical scattering and absorption. In the following, we give a simplified outline of a derivation of the relationship.

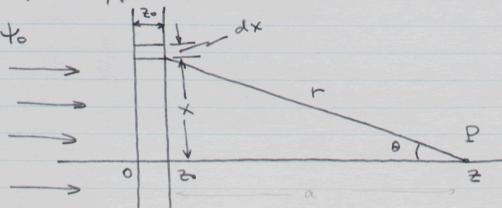
To do this, let us first consider the connection between the scattering amplitude $f(\theta, \phi)$ and the index of refraction for an electromagnetic wave passing through a scattering medium, by a method due to H. A. Lorentz. Consider an electromagnetic plane wave ψ_0 of unit amplitude impinging from vacuum on a thin slab of thickness z_0 containing N scatterers per unit volume.

$$\psi_0 = e^{i(kz-wt)}$$

Let each scatterer send out a spherical wave of amplitude

$$\psi_{sc} = f(\theta, \phi) \frac{e^{i(kr-wt)}}{r}$$

Referring to the diagram below, with $z \gg z_0$, $z_0 \ll \frac{1}{k}$, then to a first approximation:



$$\psi_p = e^{i(kz-wt)} + \int_0^\infty 2\pi x dx N z_0 \frac{f(0)}{r} e^{i(kr-wt)}$$

Since $\int x dx = r dr$

$$\psi_p = e^{i(kz-wt)} + 2\pi N z_0 e^{-iwt} \int_0^\infty dr f(0) e^{ikr}$$

To evaluate the integral above, we take $z \rightarrow \infty$ and use a convergence factor

$$\int_0^\infty dr f(0) e^{ikr} = \lim_{a^2 \rightarrow 0} \int_0^\infty dr f(0) e^{ikr} e^{-a^2 r} \approx - \frac{e^{ika}}{ik} f(0)$$

$$\text{giving } \psi_p = e^{i(kz-wt)} \left[1 + \frac{2\pi i N z_0}{k} f(0) \right]$$

Finally, we relate the above to the index of refraction (real) and absorption cross section of the material in the slab by observing that, also

$$\begin{aligned} \psi_p &= e^{i[k(z-z_0)+nkz_0-wt] - \frac{1}{2} N \sigma z_0} \\ &= e^{i(kz-wt) + i(n-1)kz_0 - \frac{1}{2} N \sigma z_0} \\ &\approx e^{i(kz-wt)} [1 + i(n-1)kz_0 - \frac{1}{2} N \sigma z_0] \end{aligned}$$

(The factor $\frac{1}{2}$ in the absorption arises because $|f|^2$ is the intensity.)

Equating the two expressions for ψ_p

$$\begin{aligned} n-1 &= \frac{2\pi N}{k^2} \operatorname{Re} f(0) \\ \sigma &= \frac{4\pi}{k} \operatorname{Im} f(0) \end{aligned} \quad \left. \right\} \quad (11)$$

The dispersion relationship is now derived by recognizing a connection between the forward scattering $\operatorname{Re} f(0)$ and the absorption. In the optical case this is perhaps most easily achieved by means of the index of refraction, which is also determined by the polarization of the medium.

$$n^2 = k = 1 + \frac{4\pi \sigma}{E} \quad (12)$$

Consider an elementary oscillator of natural frequency ω_i and absorption γ_i . The polarization and absorption are determined by the oscillator equation:

$$\frac{e}{m} \underline{E} = \ddot{\underline{r}} + \omega_i^2 \underline{r} + \gamma_i \dot{\underline{r}}$$

$$\underline{r}_i = \frac{\frac{e}{m} \underline{E}}{\omega_i^2 - \omega^2 + i\gamma_i \omega}$$

$$\underline{P}_i = \text{Re}(\epsilon \underline{r}_i) \cong \frac{e^2}{m(\omega_i^2 - \omega^2)} \underline{E}$$

for ω not too close to ω_i , and the average radiated power (absorption) is:

$$\overline{P}_i = \frac{1}{2} \epsilon \underline{E} \cdot \underline{r}_i = \frac{\frac{e^2}{m} E^2 r_i \omega^2}{(\omega_i^2 - \omega^2)^2 + \gamma_i^2 \omega^2}$$

Consider a flux $\Phi(\omega) = \frac{c}{8\pi} E^2(\omega)$ of electromagnetic energy incident on a scatterer consisting of many oscillators. We define the absorption cross-section $\sigma(\omega)$ by

$$\Phi(\omega) \sigma(\omega) = \overline{P}_i(\omega) = \int_0^\infty d\omega_i f(\omega_i) \overline{P}_i \rightarrow \frac{\pi}{2} \sigma(\omega_i - \omega)$$

A straight forward integration (for $\gamma_i \ll \omega_i$) yields.

$$\sigma(\omega) = 2\pi^2 \frac{e^2}{mc} f(\omega) \quad (13)$$

Likewise, for the polarization vector

$$\underline{D}(\omega) = N \underline{E} \int_0^\infty \frac{\frac{e^2}{m} f(\omega_i) d\omega_i}{\omega_i^2 - \omega^2} = \frac{N c \underline{E}}{2\pi^2} \int_0^\infty \frac{\sigma(\omega_i) d\omega_i}{\omega_i^2 - \omega^2}$$

Referring to eq. (13) and assuming $|n-1| \ll 1$

$$n-1 = 2\pi \frac{P}{E} = \frac{CN}{\pi} \int_0^\infty \frac{\sigma(\omega_i) d\omega_i}{\omega_i^2 - \omega^2} \quad (14)$$

Finally, equating (13) and (14), and using $\omega = kc$ and equation (11b) we have:

$$\begin{aligned} \text{Re } f(0, \omega) &= \frac{\omega^2}{2\pi^2 c} \int_0^\infty \frac{\sigma(\omega_i) d\omega_i}{\omega_i^2 - \omega^2} = \\ &= \frac{2\omega^2}{\pi} \int_0^\infty \frac{\text{Im } f(0, \omega_i) d\omega_i}{\omega_i (\omega_i^2 - \omega^2)} \end{aligned} \quad (15)$$

It is to be noted that all of the integrals above are in the sense of the "principal value", i.e., they exclude a region of width $\pm \epsilon$ on either side of ω_i and are evaluated in the limit $\epsilon \rightarrow 0$. In addition, the proper definition of the integrals in the limit $\omega \rightarrow 0$ requires that a constant, equal to $\text{Re } f(0, 0)$ be subtracted from the left side of equation (15).

In the derivation outlined above, the causality condition, eq. (15), has been derived on the basis of a specific model for the scattering and absorption of electromagnetic waves. The relativity postulate is brought into the derivation through the association of the index of refraction with the velocity of propagation in the medium ($k = n k_0$), and the connections are all made through the complex scattering amplitude in the forward direction $f(0, \omega)$ since it is only the forward scattering which is coherent with the incident radiation and, through its interference with the incident radiation, determines the propagation of the radiation through the medium.

However, despite the rather specific nature of some of the assumptions made in deriving eq. (15), the result is a general one for the propagation of any wave field, provided only that the carriers of the field (photons, pions) obey Bose-statistics. This has been proved for the electromagnetic field by Gell-Mann, Goldberger and Thirring (Phys. Rev. 95, 1612, 1954) and for finite-mass bosons by Goldberger (Phys. Rev. 99, 979, 1955) following a suggestion of Kronig (R. Kronig, Physica 12, 543, 1946) first applied by Karpplus and Ruderman (R. Karpplus and M.A. Ruderman) Phys. Rev. 98, 771, 1955). The general derivations of Goldberger et al. apply the causality condition through the quantum mechanical commutation relationship between the field amplitude operators taken at different points in space-time, by the requirement that

$$[A_\sigma(x), A_\sigma(y)] = 0 \quad \text{for } (x-y)^2 > 0 \quad (16)$$

where x and y represent four-vectors; this is equivalent to the statement that no signal can be propagated with speed greater than c .

In the following, we give a simple general derivation in which the causality condition is clearly and explicitly involved. Let us consider the time dependent scattering by a potential $V(t)$ whose Fourier transform is $V(\omega)$

$$V(t) = \int_{-\infty}^{\infty} V(\omega) e^{-i\omega t} d\omega \quad (17)$$

The scattering amplitude is obtained, in general, from the potential through a linear transformation

$$f(\omega) = K(\omega) V(\omega) \quad (18)$$

Now, suppose we send in a very narrow wave packet (δ function) which arrives at the scatterer at $t=0$; this may be expressed by the statement $V(t) = \delta(0)$. The causality condition states that for scattering in the forward direction [$f(0, \omega) \equiv F(\omega)$]

$$F(t) = 0 \quad \text{for all } t < 0 \quad (19)$$

$$\begin{aligned} \text{Now: } F(t) &= \int_{-\infty}^{\infty} F(\omega) e^{-i\omega t} d\omega = \int_{-\infty}^{\infty} K(0, \omega) V(\omega) e^{-i\omega t} d\omega = \\ &= \int_{-\infty}^{\infty} K(0, \omega) e^{-i\omega t} d\omega \int_{-\infty}^{\infty} V(t') e^{i\omega t'} dt' = \\ &= \int_{-\infty}^{\infty} K(0, \omega) e^{-i\omega t} d\omega \end{aligned}$$

Inverting, and applying eq. (19):

$$F(\omega) = K(0, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(t) e^{i\omega t} dt = \frac{1}{2\pi} \int_0^{\infty} F(t) e^{i\omega t} dt \quad (20)$$

Now, $F(t)$ which describes a real wave packet is real, so

$$\begin{aligned} \operatorname{Re} F(\omega) &= \int_0^{\infty} F(t) \cos \omega t dt \\ \operatorname{Im} F(\omega) &= \int_0^{\infty} F(t) \sin \omega t dt \end{aligned} \quad (21)$$

and the dispersion relation follows from the observation that

$$\cos \omega t = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\sin \omega t}{\omega' - \omega} d\omega'$$

through substitution into (21a) and changing the order of integration

$$\operatorname{Re} F(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\operatorname{Im} F(\omega')}{\omega' - \omega} d\omega' \quad (22)$$

This can be put into the usual form by the observation (from eq. (21b)) that

$$\operatorname{Im} F(\omega) = -\operatorname{Im} F(-\omega),$$

whence

$$\operatorname{Re} F(\omega) = \frac{2}{\pi} \int_0^{\infty} \frac{\omega' \operatorname{Im} F(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (23)$$

Finally, we observe that

$$\frac{1}{\omega'^2 - \omega^2} = \frac{\omega'^2}{\omega'^2} \frac{1}{\omega'^2 - \omega^2} + \frac{1}{\omega^2} = \frac{1}{\omega^2} \frac{1}{\omega'^2 - \omega^2} (\omega'^2 + \omega'^2 - \omega^2)$$

Substitution gives:

$$\operatorname{Re} F(\omega) = \frac{2\omega^2}{\pi} \int_0^{\infty} \frac{\operatorname{Im} F(\omega')}{\omega'(\omega'^2 - \omega^2)} d\omega' + \operatorname{Re} F(0) \quad (24)$$

Before considering the application of this relationship to scattering, we illustrate its usefulness by considering the application to a number of electro-magnetic problems, as demonstrated by Gell-Mann, Goldberger and Thirring. Let:

$$D(\omega) \equiv \operatorname{Re} F(\omega)$$

$$A(\omega) \equiv \operatorname{Im} F(\omega) = \frac{k}{4\pi} \sigma(\omega) = \frac{\omega}{4\pi c} \sigma(\omega)$$

Then, we rewrite (24):

$$D(\omega) - D(0) = \frac{\omega^2}{2\pi^2 c} \int_0^{\infty} \frac{\sigma(\omega') d\omega'}{\omega'^2 - \omega^2} \quad (25)$$

We may now obtain a useful "sum rule" by taking the limit as $\omega \rightarrow \infty$. Then, provided that

$$\frac{\sigma(\omega')}{\omega'^2} \rightarrow 0 \quad \text{faster than } \frac{1}{\omega'}, \quad \text{we have:}$$

$$D(0) - D(\infty) = \frac{1}{2\pi^2 c} \int_0^{\infty} \sigma(\omega') d\omega' \quad (26)$$

a) Consider first the scattering of a free charged particle. In this case, the scattering is frequency independent (to order e^2 at least) and

$$D(0) = D(\infty) - \frac{e^2}{mc^2}$$

Thus, calling $\sigma_0(\omega)$ the total cross section for a free charge

$$\int_0^{\infty} \sigma_0(\omega) d\omega = 0 \quad (27)$$

to order e^2 . (This is also true to order e^4)

b) Now, let the charge be bound electrically. Then $D(0) = 0$ since Rayleigh scattering $\propto k^4$, while $D(\infty) \rightarrow -\frac{e^2}{mc^2}$ for any finite binding. Thus, for a bound charge:

$$\int_0^{\infty} \sigma(\omega) d\omega = \frac{2\pi^2 e^2}{mc} \quad (28)$$

a result which we have previously is the well-known Thomas-Reiche-Kuhn dipole sum rule.

c) Finally, consider the scattering of photons from a nucleus containing Z protons and N neutrons, by applying eq. (26) to the difference between the nuclear scattering and the scattering by Z free protons and N free neutrons.

$$\begin{aligned} D_A(0) - D_A(\infty) - Z[D_p(0) - D_p(\infty)] - N[D_N(0) - D_N(\infty)] &= \\ = \frac{1}{2\pi^2 c} \int_0^{\infty} [D_A(\omega') - Z D_p(\omega') - N D_N(\omega')] d\omega' \end{aligned}$$

Now, according to the preceding,

$$D_N(0) = 0, \quad D_p(0) = -\frac{e^2}{Mc^2}, \quad D_A(0) = -\frac{Z^2 e^2}{A Mc^2}$$

furthermore, $D_A(\infty) = Z D_p(\infty) + N D_N(\infty)$

giving:

$$\frac{Nz}{A} \frac{e^2}{Mc^2} = \frac{1}{2\pi^2 c} \int_0^\infty [\sigma_A(w') - Z \sigma_p(w') - N \sigma_N(w')] dw'$$

In the absence of mesonic effects, equation (27) would apply: (29)

$$\int_0^\infty \sigma_{po}(w') dw' = \int_0^\infty \sigma_{No}(w') dw' = 0$$

giving

$$\int_0^\infty \sigma_{A0}(w') dw' = \frac{2\pi e^2}{Mc} \frac{Nz}{A} \quad (30)$$

This is the electric dipole sum rule derived by Bethe and Salinger for the case of no exchange forces (i.e. no meson effects).

However, meson effects alter this sum rule as follows: below the meson threshold, $w_t = \frac{Mc^2}{n}$, we may still apply eq. (27)

$$\int_0^{w_t} \sigma_p(w') dw' = \int_0^{w_t} \sigma_N(w') dw' = 0$$

enabling us to rewrite eq. (29)

$$\int_0^{w_t} \sigma_A(w') dw' = 2\pi^2 \left\{ \frac{Nz}{A} \frac{e^2}{Mc} + \frac{1}{2\pi^2} \int_{w_t}^\infty [Z \sigma_p + N \sigma_N - \sigma_A] dw' \right\} \quad (31)$$

The integral on the right hand side of eq. (31) has its main contribution between w_t and $\sim 2w_t$ since at high photon energies the binding of the nucleons is no longer significant. Gell-Mann, Goldberger, and Thirring have used the measured values to estimate its value; they obtain a contribution of $\approx 0.1 A \frac{e^2}{Mc}$, to within ~ 30 percent accuracy. This gives:

$$\int_0^{w_t} \sigma_A(w') dw' = 2\pi^2 \frac{Nz}{A} \frac{e^2}{Mc} \left(1 + 0.1 \frac{A^2}{Nz} \right) \quad (32)$$

It is interesting to compare this result with the electric dipole sum rule of Bethe and Salinger, who obtain,

$$\int_0^\infty \sigma_A^{ED}(w') dw' = 2\pi^2 \frac{Nz}{A} \frac{e^2}{Mc} (1 + 0.8X) \quad (33)$$

where X is the ratio of exchange to ordinary force. It is noteworthy that the right hand sides of equations (32) and (33) become equal for $X = 0.5$ with $N = Z = \frac{A}{2}$ which, subject

to some uncertainties in the derivation of eq. (33) and in values of X and the integral in eq. (31), would indicate that essentially all of the electric dipole photon absorption is contained in the energy range below the threshold for meson production. (i.e. the giant resonance)

Another application of the photon dispersion relation, considered by Gell-Mann, Goldberger and Thirring, is the derivation of certain conditions on the Compton scattering of photons by protons from the characteristics of the cross section for photo meson production on protons.

Dispersion formula

We'll obtain the Kramers-Heisenberg dispersion formula using a semi-classical method.

Let us consider an atom in an external radiation field. By effect of this field, the atom can perform transitions that we can take in account by the ordinary time-dependent perturbation method. (Cf. Schiff p. 189). Then we'll consider this quantum-mechanical system as a source of classical radiation and by use of the electric-dipole radiation formula will can obtain the differential cross section for dispersion process.

We consider only the coherent scattering case, i.e., when the initial and final states are the same and then, the scattered light has the same frequency as the incoming radiation.

Following the Schiff's treatment, we can write (in the Schiff's notation) the time-dependent wave function of the atomic system as:

$$\psi = \sum_n a_n(t) u_n e^{-iE_n t} \quad (1)$$

where u_n are the eigenfunctions of the unperturbed atom with energy eigenvalues E_n . The perturbation H' is the first order coupling term of the atomic system with a plane electromagnetic wave (which represent the incoming radiation).

$$H' = -\frac{e}{mc} \mathbf{A} \cdot \mathbf{P} \quad (2)$$

$$\text{where } \mathbf{A} = U A_0 \cos(kz - \omega t) \quad (3)$$

U is the unit vector along the polarization direction.

Taking the influence of the perturbation at first order:

$$a_n = a_n^{(0)} + a_n^{(1)} \quad (4)$$

where the a 's satisfy the equations: (Cf. Schiff. p. 190)

$$\dot{a}_n^{(0)} = 0 \quad \dot{a}_n^{(1)} = \frac{1}{i\hbar} \sum_k H'_{nk} a_k^{(0)} e^{i\omega_k t} \quad (5)$$

$$\text{where } \omega_{nk} \equiv \frac{E_n - E_k}{\hbar} \quad \text{and}$$

$$H'_{nk} = \int u_n^* H' u_k dV$$

Assuming that the system were in a definite unperturbed energy state when the perturbation is applied, we have:

$$a_k^{(0)} = \delta_{km}$$

From (5):

$$\dot{a}_n^{(1)} = \frac{1}{i\hbar} H'_{nm} e^{i\omega_m t}$$

Let us now take a stationary solution of the above equation, using (2) and (3) we have:

~~$$H'_{nk} = H'_{nm} e^{i\omega_m t}$$~~

$$H' = H^{(+) e^{-i\omega t}} + H^{(-) e^{i\omega t}}$$

where:

$$H^{(+)} \equiv -\frac{e A_0}{2mc} U e^{ik \cdot r} \cdot P$$

$$H^{(-)} \equiv -\frac{e A_0}{2mc} U e^{-ik \cdot r} \cdot P$$

$$\therefore a_n^{(1)} = -\frac{H_{nm}^{(+)}}{\hbar} \frac{e^{i(\omega_m - \omega)t}}{\omega_m - \omega} - \frac{H_{nm}^{(-)}}{\hbar} \frac{e^{i(\omega_m + \omega)t}}{\omega_m + \omega} \quad (6)$$

(Initial conditions)

$$H_{nm}^{(+)} = -\frac{e A_0}{2mc} \int u_n^* [U e^{ik \cdot r} \cdot P] u_m dV$$

$$H_{nm}^{(-)} = -\frac{e A_0}{2mc} \int u_n^* [U e^{-ik \cdot r} \cdot P] u_m dV$$

At electric dipole approximation: $e^{ik \cdot r} \approx 1$ and:

$$\int u_n^* [U \cdot P] u_m dV = i m \omega_m \int u_n^* [U \cdot r] u_m dV = i m \omega_m Z_{nm}$$

where we have taken the z axis along the polarization U and.

$$Z_{nm} = \int u_n^* Z u_m dV$$

Then:

$$H_{nm}^{(+)} = H_{nm}^{(-)} = -\frac{ie A_0}{2c} \omega_{nm} Z_{nm}$$

From (6) we have:

$$a_n^{(1)} = \frac{ie A_0}{2\hbar c} \omega_{nm} Z_{nm} e^{i\omega_m t} \left[\frac{e^{-i\omega t}}{\omega_m - \omega} + \frac{e^{i\omega t}}{\omega_m + \omega} \right]$$

The wave function is then:

$$\psi = u_m e^{-\frac{iE_m t}{\hbar}} + \frac{ie A_0}{2\hbar c} \sum_n \omega_{nm} Z_{nm} u_n \left[\frac{e^{-i\omega t}}{\omega_m - \omega} + \frac{e^{i\omega t}}{\omega_m + \omega} \right] e^{-\frac{iE_n t}{\hbar}} \quad (7)$$

We calculate now the dipole moment of the atomic system:

$$D = e \int \psi^* z \psi dV$$

Using (7) we have:

$$D = \frac{ie^2 A_0}{2\pi c} \sum_n \omega_{nm} |Z_{nm}|^2 \left[\frac{1}{\omega_{nm} + \omega} - \frac{1}{\omega_{nm} - \omega} \right] (e^{i\omega t} - e^{-i\omega t})$$

$$\therefore D = D_0 \sin \omega t$$

$$\text{where: } D_0 = \frac{2e^2 \omega A_0}{\pi c} \sum_n \frac{\omega_{nm} |Z_{nm}|^2}{\omega^2 - \omega_{nm}^2} \quad (9)$$

For an oscillating electric dipole, the intensity of radiation in the θ direction (θ is the angle between the z -axis and the observation point) is given by:

$$I(\theta) = \frac{\omega^4}{8\pi c^3} D_0^2 \sin^2 \theta$$

The intensity of the incoming radiation (calculated from the plane wave) is:

$$S = \frac{\omega^2}{8\pi c} A_0^2$$

Then the differential cross section for the process is:

$$\frac{d\Gamma(\theta)}{d\Omega} = \frac{I(\theta)}{S} = \frac{\omega^2}{A_0^2 c^2} D_0^2 \sin^2 \theta$$

Substituting the result (9) we have:

$$\frac{d\Gamma(\theta)}{d\Omega} = \left(\frac{2e^2 \omega^2}{\pi c^2} \right)^2 \left| \sum_n \frac{\omega_{nm} |Z_{nm}|^2}{\omega^2 - \omega_{nm}^2} \right|^2 \sin^2 \theta$$

This is the Kramers-Kronig dispersion formula.

Introducing the oscillator strength:

$$f_{nk} \equiv \frac{2m \omega_{nk}}{\pi} |Z_{nk}|^2$$

and the classical electronic radius

$$r_0 = \frac{e^2}{mc^2}$$

we have:

$$\frac{d\Gamma(\theta)}{d\Omega} = r_0^2 \left| \sum_n \frac{\omega^2 f_{nm}}{\omega^2 - \omega_{nm}^2} \right|^2 \sin^2 \theta$$

Variational Principles for Scattering Processes

(Lippmann and Schwinger. Phys. Rev. 79, 469, 1950)

We are concerned with the development in time of a system of two interacting parts, which are such that the interaction energy approaches zero as the two parts are separated spatially. Correspondingly, the Hamiltonian is decomposed into the unperturbed Hamiltonian H_0 , describing the two independent parts, and H_1 the energy of interaction. We want remove the time dependence associated with H_0 .

$$it \frac{\partial \Psi'(t)}{\partial t} = (H_0 + H_1) \Psi'(t) \quad (1)$$

$$\text{then: } \Psi'(t) = e^{-\frac{i}{\hbar} H_0 t} \Psi(t) \quad (2)$$

$$\therefore it \frac{\partial \Psi}{\partial t} = H_1 \Psi$$

$$\text{where: } H_1 = H_1(t) = e^{\frac{i}{\hbar} H_0 t} H_1 e^{-\frac{i}{\hbar} H_0 t} \quad (3)$$

The initially non-interacting parts are characterized by the state vector $\Psi(-\infty)$. The final state will be $\Psi(+\infty)$. This description can be made independent of the particular initial state by regarding the time development as the unfolding of a unitary transformation:

$$\begin{aligned} \Psi(t) &= U_+(t) \Psi(-\infty) \\ U_+^\dagger(t) U_+(t) &= 1 \end{aligned} \quad \} \quad (4)$$

In particular:

$$\begin{aligned} \Psi(+\infty) &= S \Psi(-\infty) \\ S &\equiv U_+(\infty) \end{aligned} \quad \} \quad (5)$$

defines the collision operator. The operator U_+ is to be obtained as solution of:

$$it \frac{\partial U_+(t)}{\partial t} = H_1(t) U_+(t) \quad (6)$$

subject to the boundary condition:

$$U_+(-\infty) = 1 \quad (7)$$

We'll introduce the unitary operator $U_-(t)$ as:

$$\Psi(t) = U_-(t) \Psi(+\infty) = U_-(t) S \Psi(-\infty) \quad (8)$$

Since the two operators are related by:

$$U_+(t) = U_-(t) S \quad (9)$$

the operator U_- is evidently the solution of:

$$i\hbar \frac{\partial U_-(t)}{\partial t} = H_1(t) U_-(t) \quad \left. \begin{array}{l} \\ \end{array} \right\} \quad (10)$$

$$U_-(\infty) = 1$$

Furthermore: $U_-(\infty) = S^{-1}$ (11)

The differential equation for U_+ can be replaced by the integral eq.

$$\begin{aligned} U_+(t) &= 1 - \frac{i}{\hbar} \int_{-\infty}^t H_1(t') U_+(t') dt' \\ &= 1 - \frac{i}{\hbar} \int_{-\infty}^t \gamma(t-t') H_1(t') U_+(t') dt' \end{aligned} \quad \left. \begin{array}{l} \\ \end{array} \right\} \quad (12)$$

which incorporates the boundary condition (7). Here:

$$\gamma(t-t') = \begin{cases} 1 & t > t' \\ 0 & t < t' \end{cases} \quad (13)$$

Similarly $U_-(t)$ obeys the integral equation:

$$\begin{aligned} U_-(t) &= 1 + \frac{i}{\hbar} \int_t^{\infty} H_1(t') U_-(t') dt' \\ &= 1 + \frac{i}{\hbar} \int_t^{\infty} dt' H_1(t') U_-(t') \gamma(t'-t) \end{aligned} \quad \left. \begin{array}{l} \\ \end{array} \right\} \quad (14)$$

By considering the limit $t \rightarrow \infty$ in (12) and $t \rightarrow -\infty$ in (14) we obtain:

$$S = 1 - \frac{i}{\hbar} \int_{-\infty}^{\infty} H_1(t) U_+(t) dt \quad (15)$$

$$S^{-1} = 1 + \frac{i}{\hbar} \int_{-\infty}^{\infty} H_1(t) U_-(t) dt \quad (16)$$

which are connected by (9)

The differential and integral equations characterizing U_+ and U_- will now be replaced by equivalent variational principles from which the fundamental equations are obtained as conditions expressing the stationary property of a suitable expression. Furthermore, the stationary value of this quantity is just S , the collision operator. Hence the variational formulation of the problem also yields a practical means of approximate calculation, since errors in the construction of S will be minimized by employing a stationary expression.

We first consider:

$$S' = U_+(\infty) - \int_{-\infty}^{\infty} U_+ \left[\frac{\partial}{\partial t} + \frac{i}{\hbar} H_1(t) \right] U_+(t) dt \quad (17)$$

which is regarded as a function of the operator $U_+(t)$, subject only to the restriction (7), and the Hermitian conjugate of the arbitrary operator $U_-(t)$. The change induced in S' by small, independent, variations of U_+ and U_- is:

$$\begin{aligned} S'S' &= (1 - U_-(\infty))^+ \delta U_+(\infty) - \\ &\quad - \int_{-\infty}^{\infty} \delta U_+^+ (t) \left[\frac{\partial}{\partial t} + \frac{i}{\hbar} H_1(t) \right] U_+(t) dt \\ &\quad + \int_{-\infty}^{\infty} \left[\left(\frac{\partial}{\partial t} + \frac{i}{\hbar} H_1(t) \right) U_-(t) \right]^+ \delta U_+(t) dt \end{aligned} \quad (18)$$

Since $I = I(U_-, U_+)$ subject to the condition (7) and then:

$$\begin{aligned} \delta I &= \delta \int_{-\infty}^{\infty} U_+^+ (\partial_t + \frac{i}{\hbar} H_1) U_+ dt = \\ &= \int_{-\infty}^{\infty} (\delta U_+^+) (\partial_t + \frac{i}{\hbar} H_1) U_+ dt + \int_{-\infty}^{\infty} U_+^+ \delta (\partial_t U_+) dt + \\ &+ \frac{i}{\hbar} \int_{-\infty}^{\infty} U_+^+ \delta (H_1 U_+) dt = \int_{-\infty}^{\infty} \delta U_+^+ (\partial_t + \frac{i}{\hbar} H_1) U_+ dt + \\ &+ |U_-^+ \delta U_+|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \delta U_+ \partial_t U_+^+ dt + \frac{i}{\hbar} \int_{-\infty}^{\infty} U_+^+ H_1 \delta U_+ dt = \\ &= \int_{-\infty}^{\infty} \delta U_+^+ (\partial_t + \frac{i}{\hbar} H_1) U_+ dt + U_-^+(\infty) \delta U_+(\infty) - \\ &- \int_{-\infty}^{\infty} \partial_t U_+^+ \delta U_+ dt + \frac{i}{\hbar} \int_{-\infty}^{\infty} H_1 U_+^+ \delta U_+ dt = \\ &= \int_{-\infty}^{\infty} \delta U_+^+ (\partial_t + \frac{i}{\hbar} H_1) U_+ dt - \int_{-\infty}^{\infty} [(2t + \frac{i}{\hbar} H_1) U_-]^+ \delta U_+ dt + \\ &+ U_+^+(\infty) \delta U_+(\infty) \end{aligned}$$

which substituted in $S'S'$ gives (18)

The requirement that S' be stationary with respect to arbitrary variations of U_+ and U_- , apart from the restriction (7), thus leads to the eqs. (6), (10) and the boundary condition (10) for U_- . It is also evident from (17) that the stationary value of S' is the collision operator S , according to (5). A somewhat more symmetrical version of (17) is:

$$\begin{aligned} S' &= \frac{1}{2} [U_+(\infty) + U_-^+(-\infty)] - \\ &- \int_{-\infty}^{\infty} \left[\frac{1}{2} U_+^+(t) \partial_t U_+(t) - \frac{1}{2} \partial_t U_+^+(t) U_+(t) + \right. \\ &\quad \left. + \frac{i}{\hbar} U_+^+(t) H_1(t) U_+(t) \right] dt \end{aligned} \quad (19)$$

subject to the restrictions:

$$U_+(-\infty) = U_-(-\infty) = 1 \quad (20)$$

It is easily verified that S' is stationary with respect to variations of U_+ and U_- about the solutions of the dif. eq. (6) and (10), subject to the boundary cond. (20), and that the stationary value of S' is S .

A variational basis for (12) and (14) is provided by:

$$\begin{aligned} S' = 1 - \frac{i}{\hbar} \int_{-\infty}^{\infty} [U_-(t) H_1(t) + H_1(t) U_+(t)] dt + \\ + \frac{i}{\hbar} \int_{-\infty}^{\infty} U_-(t) H_1(t) U_+(t) dt + \\ + \left(\frac{i}{\hbar}\right)^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_-(t) H_1(t) \gamma(t-t') H_1(t') U_+(t') dt dt' \end{aligned} \quad (21)$$

Thus:

$$\begin{aligned} S'S' = -\frac{i}{\hbar} \int_{-\infty}^{\infty} [\delta U_- + H_1 + H_1 \delta U_+] dt + \\ + \frac{i}{\hbar} \int_{-\infty}^{\infty} \delta U_- + H_1 U_+ dt + \frac{i}{\hbar} \int_{-\infty}^{\infty} U_- + H_1 \delta U_+ dt + \\ + \left(\frac{i}{\hbar}\right)^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta U_- + H_1 \gamma H_1 U_+ dt dt' + \left(\frac{i}{\hbar}\right)^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_- + H_1 \gamma H_1 \delta U_+ dt dt' \\ \therefore S'S' = \frac{i}{\hbar} \int_{-\infty}^{\infty} dt \delta U_- + H_1(t) [U_-(t) - 1 + \frac{i}{\hbar} \int_{-\infty}^{\infty} \gamma(t-t') H_1(t') U_+(t') dt'] + \\ + \frac{i}{\hbar} \int_{-\infty}^{\infty} dt [U_-(t) - 1 - \frac{i}{\hbar} \int_{-\infty}^{\infty} dt' H_1(t') U_-(t') \gamma(t'-t)] H_1(t) \delta U_+(t) \end{aligned} \quad (22)$$

which is indeed zero if U_+ and U_- satisfy their defining integral eqs. It is also evident that the stationary value of ' S' is just the ' S ', in the form (15).

This variational principle differs from (17), or (19) in that no restrictions are imposed on U_+ and U_- , and that every integral contains the interaction operator H_1 . The latter property implies that an adequate approximation to U_+ and U_- is required only during the actual process of interaction. Furthermore, the second type of variational principle will yield more accurate results than the first if the same approximate operators U_+ and U_- are employed. This is indicated by the results of inserting the simple but crude approximation:

$$U_+(t) = U_-(t) = 1 \quad (23)$$

in (17) and (21). The former yields:

$$S \approx 1 - \frac{i}{\hbar} \int_{-\infty}^{\infty} H_1(t) dt \quad (24)$$

which is equivalent to the first Born approximation, while (21) gives:

$$S \approx 1 - \frac{i}{\hbar} \int_{-\infty}^{\infty} H_1(t) dt + \left(\frac{i}{\hbar}\right)^2 \int_{-\infty}^{\infty} H_1(t) \gamma(t-t') H_1(t') dt dt' \quad (25)$$

Born
the second approx.

These approximate expressions for S illustrate a disadvantage of the variational principles thus far discussed; the unitary property is not guaranteed for an exact S . It follows from (24), for example, that:

$$S^* S \approx 1 + \frac{1}{\hbar^2} \left(\int_{-\infty}^{\infty} H_1(t) dt \right)^2 \quad (26)$$

A version of the theory that meets this objection is obtained on replacing the unitary operators $U_+(t)$ and $U_-(t)$ by:

$$V(t) = \frac{2U_+(t)}{1+S} = \frac{2U_-(t)}{1+S^{-1}} \quad (27)$$

Note that:

$$\left. \begin{aligned} V(-\infty) &= \frac{2}{1+S} \\ V(\infty) &= \frac{2}{1+S^{-1}} = \frac{2S}{1+S} \end{aligned} \right\} \quad (28)$$

$$\text{whence: } \frac{1}{2}[V(\infty) + V(-\infty)] = 1 \quad (29)$$

$$\text{and } V(\infty) = V(-\infty) \quad (30)$$

The property (29) leads us to write

$$V(\infty) = 1 - \frac{1}{2}iK ; \quad V(-\infty) = 1 + \frac{1}{2}iK \quad (31)$$

while (30) supplies the information:

$$K^+ = K^- \quad (32)$$

the so-called reaction operator K is hermitian. On remarking that

$$S = \frac{V(\infty)}{V(-\infty)} \quad (33)$$

we obtain:

$$S = \frac{1 - \frac{1}{2}iK}{1 + \frac{1}{2}iK} \quad (34)$$

which represents the unitary S in terms of the hermitian K . We shall now construct a variational principle for ' K ' in which the hermitian property is assured. Consider the operator ' K' ', defined by:

$$\begin{aligned} K' = -\frac{i}{\hbar} \int_{-\infty}^{\infty} [V^+(t) \partial_t V(t) - \partial_t V^+(t) V(t)] dt + \\ + \frac{1}{\hbar} \int_{-\infty}^{\infty} V^+(t) H_1(t) V(t) dt + \\ + \frac{i}{2} [V(\infty) - V(-\infty)] - \frac{i}{2} [V^+(\infty) - V^+(-\infty)] \end{aligned} \quad (35)$$

which is evidently hermitian for arbitrary $V(t)$. The effect of a small variation in $V(t)$ and $V^+(t)$ is indicated by:

$$\delta' K' = -\frac{1}{\hbar} \int_{-\infty}^{\infty} \left\{ \delta V^+(t) [i\hbar \partial_t - H_1(t)] V(t) + [(i\hbar \partial_t - H_1(t)) V(t)]^\dagger \delta V(t) \right\} dt - \frac{i}{2} \left\{ [V^+(\infty) - V^+(-\infty)] \delta \left(\frac{V(\infty) + V(-\infty)}{2} \right) + \right. \\ \left. + \left(\frac{V^+(\infty) + V^+(-\infty)}{2} - 1 \right) \delta [V(\infty) - V(-\infty)] - \delta \left(\frac{V^+(\infty) + V^+(-\infty)}{2} \right) [V(\infty) - V(-\infty)] - \delta [V^+(\infty) - V^+(-\infty)] \left(\frac{V(\infty) + V(-\infty)}{2} - 1 \right) \right\} \quad (36)$$

If, therefore, $V(t)$ is restricted by the mixed boundary condition (29), ' K' is stationary with respect to variations about the solution of the differential equation:

$$[i\hbar \frac{\partial}{\partial t} - H_1(t)] V(t) = 0 \quad (37)$$

and the stationary value of ' K' equals K , according to (31) and (32).

The integral equation satisfied by $V(t)$ can be constructed from that obeyed by $V^+(t)$, or directly in the following manner. On integrating the differential equation (37) from $-\infty$ to t , and from ∞ to t , we obtain

$$\left. \begin{aligned} V(t) &= V(-\infty) - \frac{i}{2\hbar} \int_{-\infty}^t H_1(t') V(t') dt' \\ V(t) &= V(\infty) + \frac{i}{2\hbar} \int_t^{\infty} H_1(t') V(t') dt' \end{aligned} \right\} \quad (38)$$

The addition of these equations yields, in consequence of the boundary condition (29):

$$V(t) = 1 - \frac{i}{2\hbar} \int_{-\infty}^{\infty} \epsilon(t-t') H_1(t') V(t') dt' \quad (39)$$

where: $\epsilon(t-t') = \begin{cases} 1 & t > t' \\ -1 & t < t' \end{cases}$ (40)

Conversely, the differential equation and boundary condition obeyed by $V(t)$ can be deduced from the integral equation. Note that

$$K = i [V(\infty) - V(-\infty)] = \frac{1}{\hbar} \int_{-\infty}^{\infty} H_1(t) V(t) dt \quad (41)$$

A variational principle formulation of this integral equation is provided by the expression

$$\begin{aligned} K' &= \frac{1}{\hbar} \int_{-\infty}^{\infty} [H_1(t) V(t) + V^+(t) H_1(t)] dt - \\ &- \frac{1}{\hbar} \int_{-\infty}^{\infty} V^+(t) H_1(t) V(t) dt - \\ &- \frac{i}{2\hbar^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} V^+(t) H_1(t) \epsilon(t-t') H_1(t') V(t') dt dt' \end{aligned} \quad (42)$$

which is obviously hermitian for arbitrary $V(t)$. Now,

$$\begin{aligned} \delta' K' &= -\frac{1}{\hbar} \int_{-\infty}^{\infty} \delta V^+(t) H_1(t) [V(t) - 1 + \frac{i}{2\hbar} \int_{-\infty}^{\infty} \epsilon(t-t') H_1(t') V(t') dt'] dt \\ &- \frac{1}{\hbar} \int_{-\infty}^{\infty} [V(t) - 1 + \frac{i}{2\hbar} \int_{-\infty}^{\infty} \epsilon(t-t') H_1(t') V(t') dt']^\dagger H_1(t) \delta V(t) dt \end{aligned} \quad (43)$$

which is indeed zero if $V(t)$ satisfies the integral equation (39). Furthermore, the stationary value of ' K' is just (41), the correct reaction operator.

The abstract theory thus far developed can be made more explicit by introducing eigenfunctions, Φ_a , for the separated parts of the system, which will describe the initial and final states. Thus, since $S\Phi_a$ is the total final state that emerges from the initial state Φ_a , the probability that the system will be found eventually in the particular state Φ_b , is

$$W_{ba} = |(\Phi_b, S\Phi_a)|^2 = |S_{ba}|^2 \quad (44)$$

It is slightly more convenient to deal with the operator

$$T = S - 1 \quad (45)$$

which generates the change in the state vector produced by the interaction process. The unitary property of S implies that

$$T^+ T = -(T + T^+) \quad (46)$$

and the probability that the system will be found in a particular final state differing from the initial one is:

$$b \neq a ; \quad W_{ba} = |T_{ba}|^2 \quad (47)$$

Now, according to (15):

$$T = -\frac{i}{\hbar} \int_{-\infty}^{\infty} H_1(t) U_+(t) dt$$

and: $T_{ba} = -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt (\Phi_b, H_1(t) U_+(t) \Phi_a)$

$$= -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt (\Phi_b, e^{\frac{i}{\hbar} H_0 t} H_1 e^{-\frac{i}{\hbar} H_0 t} U_+(t) \Phi_a) \quad (48)$$

according to eq. (3).

It should be noted that Φ_b cannot be an exact eigenfunction of H_0 , since a superposition of momentum states (wave packet) is required to produce the spatial localizability involved in the definite expansion of the two parts of the system. An equivalent description is obtained, however, by introducing eigenfunctions of H_0 :

$$H_0 \phi_b = E_b \phi_b \quad (49)$$

and simulating the cessation of interaction, arising from the separation of the component parts of the system, by an adiabatic decrease in the interaction strength as $t \rightarrow \pm\infty$. The latter can be represented by the factor $e^{-\frac{\epsilon}{\hbar} |t|}$ where ϵ is arbitrarily small. Accordingly, (48) becomes:

$$\begin{aligned} T_{ba} &= -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt (\phi_b, e^{\frac{i}{\hbar} H_0 t} H_1 e^{-\frac{i}{\hbar} H_0 t} U_+(t) \phi_a) = \\ &= -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt (e^{\frac{i}{\hbar} H_0 t} H_1 e^{-\frac{i}{\hbar} H_0 t} \phi_b, U_+(t) \phi_a) = \\ &= -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt (e^{\frac{i}{\hbar} H_0 t} H_1 e^{-\frac{i}{\hbar} E_0 t} \phi_b, U_+(t) \phi_a) = \\ &= -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt (\phi_b, e^{\frac{i}{\hbar} E_0 t} H_1 e^{-\frac{i}{\hbar} H_0 t} U_+(t) \phi_a) \end{aligned}$$

Substituting: $H_1 \rightarrow H_1 e^{-\frac{\epsilon}{\hbar} |t|} \rightarrow H_1 e^{\frac{i}{\hbar} (E_b - H_0)t}$

$$\begin{aligned} T_{ba} &= -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt (\phi_b, H_1 e^{\frac{i}{\hbar} (E_b - H_0)t} e^{-\frac{\epsilon}{\hbar} |t|} U_+ \phi_a) = \\ &= -\frac{i}{\hbar} (\phi_b, H_1 \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar} (E_b - H_0)t} e^{-\frac{\epsilon}{\hbar} |t|} U_+ \phi_a) \end{aligned}$$

Then:

$$T_{ba} = -\frac{i}{\hbar} (\phi_b, H_1 \psi_a^{(+)}(E_b)) \quad (50)$$

where:

$$\psi_a^{(+)}(E) \equiv \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar} (E - H_0)t} e^{-\frac{\epsilon}{\hbar} |t|} U_+(t) \phi_a \quad (51)$$

Formula (16) for $S^- - 1 = T^+$ leads, in a similar way, to:

$$(T^+)_{bc} = \frac{i}{\hbar} (\phi_b, H_1 \psi_a^{(-)}(E_b)) \quad (52)$$

or equivalently,

$$T_{ab} = -\frac{i}{\hbar} (\psi_a^{(-)}(E_b), H_1 \phi_b) \quad (53)$$

in which:

$$\psi_a^{(-)}(E) = \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar} (E - H_0)t} e^{-\frac{\epsilon}{\hbar} |t|} U_-(t) \phi_a \quad (54)$$

Determining equations for $\psi_a^{(+)}(E)$ and $\psi_a^{(-)}(E)$ can be obtained from (12) and (14), the integral equations for U_+ and U_- . Thus:

$$\begin{aligned} \psi_a^{(+)}(E) &= \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar} (E - H_0)t} e^{-\frac{\epsilon}{\hbar} |t|} \phi_a - \\ &\quad - \frac{i}{\hbar} \int_{-\infty}^{\infty} dt dt' e^{\frac{i}{\hbar} (E - H_0)t} e^{-\frac{\epsilon}{\hbar} |t|} \gamma(|t-t'|) H_1(t') U_+(t') dt' \end{aligned}$$

the second integral on right side is:

$$\begin{aligned} &\int_{-\infty}^{\infty} dt dt' e^{\frac{i}{\hbar} (E - H_0)t} e^{-\frac{\epsilon}{\hbar} |t|} \gamma(t+t') e^{\frac{i}{\hbar} H_0 t'} H_1 e^{-\frac{i}{\hbar} H_0 t'} U_+(t') dt' dt \\ &= \int_{-\infty}^{\infty} dt dt' e^{\frac{i}{\hbar} E t} e^{-\frac{i}{\hbar} H_0(t-t')} H_1 e^{-\frac{i}{\hbar} (|t|+|t'|)} e^{-\frac{i}{\hbar} H_0 t'} e^{-\frac{i}{\hbar} H_0 t'} U_+(t') \gamma(t-t') \end{aligned}$$

Introducing the variable: $z = |t-t'|$, we have:

$$\begin{aligned} &\int_{-\infty}^{\infty} dz dt' e^{\frac{i}{\hbar} E(z+t')} e^{-\frac{i}{\hbar} H_0 z} H_1 e^{-\frac{i}{\hbar} (z+2|t'|)} e^{-\frac{i}{\hbar} H_0 t'} U_+(t') \gamma(z) = \\ &= \int_0^{\infty} dz e^{\frac{i}{\hbar} (E-H_0)z} e^{-\frac{\epsilon z}{\hbar}} \int_{-\infty}^{\infty} dt' e^{\frac{i}{\hbar} (E-H_0)t'} e^{-\frac{\epsilon}{\hbar} |t'|} U_+(t') \end{aligned}$$

From eq. (51) we have as final result for $\psi_a^{(+)}(E)$:

$$\begin{aligned} \psi_a^{(+)}(E) &= \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar} (E-E_b)t} e^{-\frac{\epsilon}{\hbar} |t|} \phi_a - \\ &\quad - \frac{i}{\hbar} \int_0^{\infty} dz e^{\frac{i}{\hbar} (E-H_0)z} e^{-\frac{\epsilon z}{\hbar}} H_1 \psi_a^{(+)}(E) \end{aligned} \quad (55)$$

and in a similar way:

$$\begin{aligned} \psi_a^{(-)}(E) &= \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar} (E-E_b)t} e^{-\frac{\epsilon}{\hbar} |t|} \phi_a + \\ &\quad + \frac{i}{\hbar} \int_0^{\infty} dz e^{\frac{i}{\hbar} (E-H_0)z} e^{-\frac{\epsilon z}{\hbar}} H_1 \psi_a^{(-)}(E) \end{aligned} \quad (56)$$

where $z = |t-t'|$. Now

$$\begin{aligned} &\int_0^{\infty} dz e^{\frac{i}{\hbar} (E-H_0)z} e^{-\frac{\epsilon z}{\hbar}} = \frac{1}{E + i\epsilon - H_0} = \\ &= \frac{E - H_0}{(E - H_0)^2 + \epsilon^2} + \frac{i\epsilon}{(E - H_0)^2 + \epsilon^2} = P \frac{1}{E - H_0} + i\pi \delta(E - H_0) \end{aligned} \quad (57)$$

The last expression is a symbolic statement of the following integral properties possessed by the real and imaginary parts of (57) in the limit as $\epsilon \rightarrow 0$:

$$\lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \frac{x}{x^2 + \epsilon^2} f(x) dx = P \int_{-\infty}^{\infty} \frac{f(x)}{x} dx \quad (58)$$

$$\lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\epsilon}{x^2 + \epsilon^2} f(x) dx = f(0)$$

where P denotes the principal part of the integral and $f(x)$ is an arbitrary function. Therefore:

$$\psi_a^{(\pm)}(E) = 2\pi \hbar \delta(E - E_a) \phi_a + \frac{1}{E \pm i\epsilon - H_0} H_1 \psi_a^{(\pm)}(E) \quad (59)$$

and, on writing:

$$\psi_a^{(\pm)}(E) = 2\pi \hbar \delta(E - E_a) \psi_a^{(\pm)} \quad (60)$$

we obtain:

$$\psi_a^{(\pm)} = \phi_a + \frac{1}{E_a \pm i\epsilon - H_0} H_1 \psi_a^{(\pm)} \quad (61)$$

These equations provide a time-independent formulation of the scattering problem, in which the small positive or negative imaginary addition to the energy serves to select, automatically, outgoing or incoming scattered waves.

A matrix element of the operator T can now be expressed as:

$$T_{ba} = -2\pi i \delta(E_a - E_b) T_{ba} \quad (62)$$

where: $T_{ba} = (\phi_b, H_1 \psi_a^{(+)}) = (\psi_b^{(-)}, H_1 \phi_a) \quad (63)$

are equivalent forms for an element of the association matrix \mathbb{T} , which is defined only for states of equal energy. The resulting formula for the transition probability,

$$W_{ba} = 4\pi^2 [\delta(E_a - E_b)]^2 |T_{ba}|^2 \quad (64)$$

is to be interpreted by replacing one factor $\delta(E_a - E_b)$ by its defining time integral:

$$\delta(E_a - E_b) = \frac{1}{2\pi \hbar} \int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(E_a - E_b)t} - e^{i\epsilon t} \frac{dt}{t} \quad \epsilon \rightarrow 0 \quad (65)$$

in which $E_a - E_b$ must be placed equal to zero in view of the second delta-function factor. The expression thus obtained

$$W_{ba} = \frac{2\pi}{\hbar} \delta(E_a - E_b) |T_{ba}|^2 \int_{-\infty}^{\infty} dt \quad (66)$$

evidently describes the fact that transition occurs only between states of equal energy for the repeated system, and with an intensity proportional to the total time of effective interaction. In the idealized limit $\epsilon \rightarrow 0$ the latter is infinitely large. However, we infer from (66) that the rate at which the transition probability increases is:

$$W'_{ba} = \frac{2\pi}{\hbar} \delta(E_a - E_b) |T_{ba}|^2 \quad (67)$$

A somewhat more satisfactory derivation of this result follows from the evaluation of:

$$W_{ba} = \frac{\partial}{\partial t} |(\phi_b, U(t) \phi_a)|^2 \quad (68)$$

which express the increase, per unit time, of the probability that the

system, known to be initially in the state a , will be found at time t in the state b . The result is, of course, the same (67) as we can check easily.

A simple expression for the total rate of transition from the initial state follows from the general property of the operator T contained in (46). On writing a matrix element of this operator relation and substituting (62) we obtain

$$4\pi^2 \sum_b \delta(E_a - E_b) T_{ba}^* \delta(E_b - E_c) T_{bc} = 2\pi i \delta(E_a - E_c) (T_{ac} - T_{ca}^*) \quad (69)$$

The factor $\delta(E_a - E_c)$ can be canceled and (69) then yields, for the special situation, $c=a$

$$4\pi^2 \sum_b \delta(E_a - E_b) |T_{ba}|^2 = -4\pi \text{Im}(T_{aa}) \quad (70)$$

or: $\sum_b W_{ba} = -\frac{2}{\hbar} \text{Im}(T_{aa}) \quad (71)$

The left side of this formula is not exactly the total rate of transition out of the state a , since $b=a$ is included in the summation. However, a single state makes no contribution to such a summation; a group of states is required. A relation of the type (71) is characteristic of a wave theory, in which the reduction in intensity of a plane wave passing through a scattering medium is accounted for by destructive interference between the original wave and the secondary waves scattered in the direction of propagation.

A variational formulation of eq. (61) by means of a stationary expression for T_{ba} can be obtained from the variational principle (21). A matrix element of this operator equation reads: (remember the eq. (3))

$$\begin{aligned} T_{ba} &= -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt [e^{\frac{i}{\hbar}(E_a - H_0)t} U_-(t) \phi_b, H_1 \phi_a] + \\ &\quad + (\phi_b, H_1 e^{\frac{i}{\hbar}(E_b - H_0)t} U_+(t) \phi_a)] + \\ &\quad + \frac{i}{\hbar} \int_{-\infty}^{\infty} dt [e^{-\frac{i}{\hbar}H_0 t} U_-(t) \phi_b, H_1 e^{-\frac{i}{\hbar}H_0 t} U_+(t) \phi_a] \\ &\quad + \left(\frac{i}{\hbar} \right)^2 \int_{-\infty}^{\infty} dt \int_{-\infty}^t dt' [e^{-\frac{i}{\hbar}H_0 t} U_-(t) \phi_b, H_1 e^{-\frac{i}{\hbar}H_0(t-t')} \times \\ &\quad \times H_1 e^{-\frac{i}{\hbar}H_0 t'} U_+(t') \phi_a] \end{aligned} \quad (72)$$

in which the adiabatic reduction of H_1 for large $|t|$ has not been indicated explicitly. We now restrict ourselves to the class of stationary states, according to the assumption:

$$e^{-\frac{i}{\hbar} H_0 t} U \pm(t) \phi_a = e^{-\frac{i}{\hbar} E a t} \psi_a^{(\pm)} \quad (73)$$

The result of performing the time integration is expressed by:

$$\begin{aligned} T'_{ba} &= (\psi_b^{(+)}, H_1 \phi_a) + (\phi_b, H_1 \psi_a^{(+)}) - (\psi_b^{(-)}, H_1 \psi_a^{(+)}) + \\ &+ (\psi_b^{(-)}, H_1 \frac{1}{E+i\epsilon-H_0} H_1 \psi_a^{(+)}) \end{aligned} \quad (74)$$

where E is the common energy of states a and b . We shall verify directly that (74) has the required properties. Thus:

$$\begin{aligned} S^* T'_{ba} &= (\delta \psi_b^{(-)}, H_1 [\phi_a + \frac{1}{E+i\epsilon-H_0} H_1 \psi_a^{(+)} - \psi_a^{(+)})] + \\ &+ (\phi_b + \frac{1}{E-i\epsilon-H_0} H_1 \psi_b^{(-)} - \psi_b^{(-)}, H_1 S \psi_a^{(+)}) \end{aligned} \quad (75)$$

which is indeed zero for variations about the solutions of (61). Furthermore, it is a consequence of the latter equations that:

$$\begin{aligned} (\psi_b^{(-)}, H_1 \psi_a^{(+)}) - (\psi_b^{(-)}, H_1 \frac{1}{E+i\epsilon-H_0} H_1 \psi_a^{(+)}) &= \\ &= (\psi_b^{(-)}, H_1 \phi_a) = (\psi_b, H_1 \psi_a^{(+)}) \end{aligned} \quad (76)$$

so that the stationary value of T'_{ba} is T_{ba} , according to (63).

A similar theory can be developed for the matrix elements of the operator K . It is easily shown that

$$K_{ba} = 2\pi \delta(E_a - E_b) K_{ba} \quad (77)$$

where: $K_{ba} = (\phi_b, H_1 \psi_a^{(1)}) = (\psi_b^{(1)}, H_1 \phi_a)$ (78)

~~Additional steps will be required here.~~ The time-independent state vector $\psi_a^{(1)}$ describes a stationary state, according to the relation:

$$e^{-\frac{i}{\hbar} H_0 t} V(t) \phi_a = e^{-\frac{i}{\hbar} E a t} \psi_a^{(1)} \quad (79)$$

and obeys the equation:

$$\psi_a^{(1)} = \phi_a + P \left(\frac{1}{E_a - H_0} \right) H_1 \psi_a^{(1)} \quad (80)$$

A variational basis for (78) and (80) is provided by:

$$\begin{aligned} K'_{ba} &= K'_{ab}^* = (\psi_b^{(1)}, H_1 \phi_a) + \\ &+ (\phi_b, H_1 \psi_a^{(1)}) - (\psi_b^{(1)}, H_1 \psi_a^{(1)}) + \\ &+ (\psi_b^{(1)}, H_1 P \left[\frac{1}{E - H_0} \right] H_1 \psi_a^{(1)}) \end{aligned} \quad (81)$$

The connection between the matrices T and K is obtained from

$$T = S - 1 = \frac{-iK}{1 + \frac{1}{2}iK} \quad (82)$$

or rewriting the latter as:

$$T + \frac{1}{2}iKT = -iK \quad (83)$$

Non-vanishing matrix elements of this operator relation are restricted to states of equal energy, according to (62) and (77), whence

$$T_{ba} + i\pi \sum_c K_{bc} \delta(E_c - E) T_{ca} = K_{ba} \quad (84)$$

where E is the common energy states a and b (E_a). An effective way to solve this equation is to construct the eigenfunctions of K , which are defined by the eigenvalue equation:

$$\sum_a K_{ba} \delta(E_a - E) f_{aA} = K_A f_{bA} \quad (85)$$

~~These basis elements of K can be exhibited in terms of the displacement basis.~~ Since K is an Hermitian matrix, the eigenvalues K_A are real, the eigenfunctions f_{aA} are orthogonal, and may be normalized according to:

$$\sum_a f_{aA}^* \delta(E_a - E) f_{aB} = \delta_{AB} \quad (86)$$

The matrix elements of K can be exhibited in terms of the eigenfunctions and eigenvalues of K :

$$K_{ba} = \sum_A f_{bA} K_A f_{aA}^* \quad (87)$$

Equation (84) for T will then be satisfied by:

$$T_{ba} = \sum_A f_{bA} T_A f_{aA}^* \quad (88)$$

where $T_A + i\pi K_A T_A = K_A$ (89)

or $T_A = \frac{K_A}{1 + i\pi K_A}$ (90)

This is only to say that T is a function of K and therefore possesses the same eigenfunctions, while its eigenvalues are determined by those of K . These eigenvalues can be conveniently expressed by introducing the real angles δ_A , according to

$$K_A = -\frac{1}{\pi} \tan \delta_A \quad (91)$$

so that: $T_A = -\frac{1}{\pi} \sin \delta_A e^{i\delta_A}$ (92)

The resulting expression for the transition probability per unit time is:

$$w_{ba} = \frac{2}{\pi h} \left| \sum_A \sin \delta_A e^{i\delta_A} f_{ba} f_{AA}^* \right|^2 \delta(E_a - E_b) \quad (93)$$

and the total probability per unit time for transitions from a particular state is given by:

$$\sum_b w_{ba} = \frac{2}{\pi h} \sum_A \sin^2 \delta_A |f_{AA}|^2 \quad (94)$$

according to (93) or (71). Finally, the sum of the total transition probability per unit time over all initial states of the same energy is expressed by:

$$\sum_b w_{ba} \delta(E_a - E) = \frac{2}{\pi h} \sum_A \sin^2 \delta_A \quad (95)$$

These results are generalizations of familiar formulas obtained in the conventional phase shift analysis of the scattering of a particle by a central field of force. In the latter situation, the eigenfunctions of \mathbf{K} are evident from symmetry considerations, namely the invariance of K_{ba} under a simultaneous rotation of \mathbf{k}_a and \mathbf{k}_b , the propagation vectors that define the initial and final states. It may be inferred that the f_{AA} are spherical harmonics, considered as a function of the angles that define the direction of \mathbf{k}_A ,

$$f_{AA} = C Y_{lm}(\mathbf{k}_A); \quad A = l, m \quad (96)$$

and that the eigenvalues of \mathbf{K} depend only upon the order of the spherical harmonics, i.e., $\delta_A \equiv \delta_l$. The constant C is fixed by the normalization convention contained in (86) which now reads,

$$|C|^2 \int Y_{l,m}^*(\mathbf{k}) Y_{l,m}(\mathbf{k}) g d\Omega = 2\pi \delta_{lm} \quad (97)$$

Here $g d\Omega$ is the number of states, per unit energy range, associated with motion within the solid angle $d\Omega$. This occurs as a weight factor in a summation over all states as restricted by the factor $\delta(E_a - E)$. Explicitly,

$$g = \frac{p^2 dp}{8\pi^3 t^3 dE} = \frac{1}{8\pi^3 t} \frac{k^2}{v} \quad (98)$$

if we consider a unit spatial volume. The second form in (98) expresses g in terms of the wave number k and v , the speed of the particle. With spherical harmonics that are normalized on a unit sphere, (97) requires that:

$$|C|^2 = \frac{1}{g} = \frac{8\pi^3 t v}{k^2} \quad (99)$$

We may now compute from (93) the probability, per unit time, that

the particle is scattered from the direction of \mathbf{k}_a into the solid angle $d\Omega$ around the direction of \mathbf{k}_b

$$w = \frac{2}{\pi h} \left| \sum_{l,m} \sin \delta_l e^{i\delta_l} |C|^2 Y_{lm}(\mathbf{k}_b) Y_{lm}^*(\mathbf{k}_a) \right|^2 g d\Omega$$

We then obtain the well-known expression of the differential cross section for scattering through an angle θ ,

$$dP(\theta) = \frac{1}{k^2} \left| \sum_l (2l+1) \sin \delta_l e^{i\delta_l} P_l(\cos \theta) \right|^2 d\Omega \quad (100)$$

or dividing w by v , which measures the flux of incident particles, and employing the spherical harmonics addition theorem:

$$\sum_{l,m} Y_{lm}(\mathbf{k}_b) Y_{lm}^*(\mathbf{k}_a) = \frac{2l+1}{4\pi} P_l(\cos \theta) \quad (101)$$

where the Legendre polynomial $P_l(\cos \theta)$ is a function of θ , the angle between \mathbf{k}_a and \mathbf{k}_b . The total scattering cross section is obtained from (94):

$$\begin{aligned} \sigma &= \frac{2}{\pi h v} \sum_{l,m} \sin^2 \delta_l |C|^2 |Y_{lm}(\mathbf{k}_a)|^2 = \\ &= \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l \end{aligned} \quad (102)$$

in consequence of (101). Since the total cross section is independent of the incident direction, the same result follows immediately from (95).

We consider finally, the variational formulation of problems possessing the general character of the scattering by a central force field; namely, those in which the eigenfunctions of \mathbf{K} are determined by symmetry considerations, and the basic question is to obtain the eigenvalues K_{AB} or the phase angles δ_{AB} . For this purpose, we notice that the inverse of (87) is

$$\sum_{b,a} f_{bb}^* \delta(E_b - E) K_{bab} \delta(E_a - E) = K_A \delta_{AB} \quad (103)$$

On introducing the state vectors

$$\sum_a \phi_a f_{AA} \delta(E_a - E) = \phi_A \quad (104)$$

and:

$$\sum_a \psi_a^{(1)} f_{AA} \delta(E_a - E) = \psi_A^{(1)} \quad (105)$$

the variational principle (81) becomes:

$$\begin{aligned} -\frac{1}{\pi} \tan \delta_A' \delta_{AB} &= (\psi_B^{(1)}, H_1 \phi_A) + (\phi_B, H_1 \psi_A^{(1)}) - \\ &- (\psi_B^{(1)}, H_1 \psi_A^{(1)}) + (\psi_B^{(1)}, H_1 P \left[\frac{1}{E - H_0} \right] H_1 \psi_A^{(1)}) \end{aligned} \quad (106)$$

Note that ϕ_A , or more exactly written $\phi_{A,E}$, has the following orthogonality-normalization property:

$$(\phi_{A,E}, \phi_{B,E'}) = \sum_a f_{AA}^* \delta(E_a - E) f_{AB} \delta(E_a - E') = \\ = \delta(E - E') \sum_a f_{AA}^* \delta(E_a - E) f_{AB} = \delta_{AB} \delta(E - E') \quad (107)$$

and that the inverses of (104) and (105) are:

$$\phi_A = \sum_a f_{AA}^* \phi_A \quad (108)$$

$$\psi_A^{(1)} = \sum_a f_{AA}^* \psi_A^{(1)} \quad (109)$$

which are expansions of these state vectors in eigenvectors of K .

General Theory of Scattering Processes (Seminar Lecture by J. Schwinger, 1947)

We assume we are dealing with a system whose Hamiltonian is:

$$H = H_0 + V$$

We know the eigenstates of H_0 . V is not necessarily small compared to H_0 . We are looking for a stationary state solution corresponding to an energy E , where E lies in the continuous spectrum of the operator H_0 .

$$H\psi = (H_0 + V)\psi = E\psi$$

$$\text{or: } (E - H_0)\psi = V\psi$$

We solve this for:

$$\psi = \frac{1}{E - H_0} V\psi + \phi$$

where the first term is a particular solution and the second, the solution of the homogeneous eq., i.e.

$$H_0\phi = E\phi$$

The ψ we get will depend upon which $\phi = \phi_A$ we start out with, so we associate solutions ψ_A of $H\psi_A = E\psi_A$ with solutions ϕ_A of $H_0\phi_A = E\phi_A$

Since E is one of the eigenvalues in the continuous spectrum of H_0 , the operator $(E - H_0)^{-1}$ is undefined. We therefore imagine E possessing a slight imaginary part.

$$E = E_0 + \frac{i\gamma}{2}$$

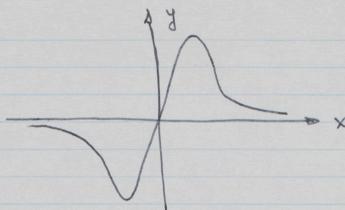
This formal trick is equivalent to the (more cumbersome) introduction of wave-packets. It will turn out $\gamma > 0$ leads to outgoing waves, $\gamma < 0$ to incoming waves, so $\gamma > 0$ is the proper choice for scattering problems.

$$\therefore (E - H_0)^{-1} = (E_0 - H_0 + \frac{i\gamma}{2})^{-1} = \frac{E_0 - H_0 - i\frac{\gamma}{2}}{(E_0 - H_0)^2 + (\frac{\gamma}{2})^2}$$

We are interested in the limit of this expression as γ approaches zero.

Real part:

$$y = \frac{x}{x^2 + (\frac{r}{2})^2}$$

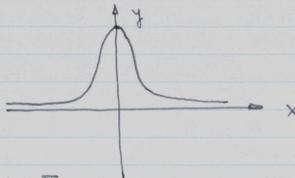


$$\int_{-\infty}^{\infty} \frac{x}{x^2 + (\frac{r}{2})^2} f(x) dx = \left(\int_{-\infty}^{-\epsilon} + \int_{\epsilon}^{\infty} + \int_{-\epsilon}^{\epsilon} \right) \frac{x}{x^2 + (\frac{r}{2})^2} f(x) dx$$

$$\therefore \int_{-\infty}^{\infty} \frac{x}{x^2 + (\frac{r}{2})^2} f(x) dx \rightarrow P \int_{-\infty}^{\infty} \frac{1}{x} f(x) dx \quad (P \text{ = principal value})$$

Imaginary part:

$$y = \frac{\frac{r}{2}}{x^2 + (\frac{r}{2})^2}$$



$$\text{Since: } \int_{-\infty}^{\infty} \frac{\frac{r}{2}}{x^2 + (\frac{r}{2})^2} dx = \pi$$

$$\int_{-\infty}^{\infty} \frac{\frac{r}{2}}{x^2 + (\frac{r}{2})^2} f(x) dx \rightarrow \pi \int_{-\infty}^{\infty} \delta(x) f(x) dx \quad r \rightarrow 0$$

Therefore:

$$\lim_{r \rightarrow 0} (E_0 - H_0 + \frac{i r}{2})^{-1} = P \left(\frac{1}{E_0 - H_0} \right) - \pi i \delta(E_0 - H_0)$$

Later on we will try to interpret this result physically. We now return to consideration of:

$$\psi_a = \phi_b + \frac{1}{E_a - H_0} V \phi_a$$

We expand ψ_a in terms of eigenfunctions ϕ_b of H_0 :

$$S_{ba} = (\phi_b, \psi_a) / E(\phi_b) \quad \psi_a = \sum_b \phi_b S_{ba}$$

$$S_{ba} = (\phi_b, \psi_a) = (\phi_b, \phi_a) + (\phi_b, \frac{1}{E_a - H_0} V \phi_a)$$

$$\text{But: } (\phi_b, \frac{1}{E_a - H_0} V \phi_a) = (\frac{1}{E_a^* - H_0} \phi_b, V \phi_a) = \frac{1}{E_a^* - E_b} (\phi_b, V \phi_a)$$

The matrix $T_{ba} \equiv (\phi_b, V \phi_a)$

which occurs here will be of importance throughout this analysis. T_{ba} is the generalization of the "matrix-element" $V_{ba} \equiv (\phi_b, V \phi_a)$, which is used in the Born approximation.

For $b \neq a$, we get:

$$|S_{ba}|^2 = \frac{1}{(E_a - E_b)^2 + (\frac{r}{2})^2} |T_{ba}|^2$$

and in the limit r very small:

$$|S_{ba}|^2 \rightarrow \frac{2\pi}{r} \delta(E_a - E_b) |T_{ba}|^2$$

To interpret this, we remember that we are dealing with complex energies. So the wave-functions have a time-factor $\exp(-\frac{i}{\hbar} Et) = \exp(-\frac{i}{\hbar} E_0 t + \frac{K}{2\pi} t)$

So the square of a wave-function has the time-factor $\exp(\frac{K}{2\pi} t)$; it therefore increases in time provided $r > 0$.

This corresponds to the physical interpretation in terms of wave-packets - a packet of incident plane waves, and slowly accumulating probability of finding outgoing (scattered) spherical waves. Including the time-factor explicitly, we get ($b \neq a$)

$$|S_{ba}|^2 = \frac{2\pi}{r} \delta(E_a - E_b) |T_{ba}|^2 \exp(\frac{r}{\hbar} t)$$

Now $|S_{ba}|^2$ represents the probability of finding state ϕ_b present in a measurement upon the system in state ϕ_a . This probability increases with time. Its time rate of change is:

$$\frac{d}{dt} |S_{ba}|^2 = \frac{2\pi}{\hbar} \delta(E_a - E_b) |T_{ba}|^2 = w_{ba}$$

where we have passed to the limit $r \rightarrow 0$.

We get the Born approximation from this rigorous result if we replace $T_{ba} = (\phi_b, V \phi_a)$ by the matrix-element $V_{ba} = (\phi_b, V \phi_a)$.

Time-reversal

We shall want to construct a variational principle for the matrix elements T_{ba} . Since we are working with complex energies, the operators are not Hermitian, and we are therefore concerned with finding Hermitian adjoints. Clearly the adjoint is obtained by letting r go into $-r$ everywhere. But this operation is equivalent to preserving r , but letting t go into $-t$ everywhere. We are therefore naturally.

led to investigation of the operation of time-reversal.

If $H\psi_a = E\psi_a$ then $H^*\psi_a^* = E^*\psi_a^*$
(H^* = complex conjugate, not hermitian adjoint). Now in many cases one can find a matrix U such that $H^* = UHU^{-1}$

Example: Dirac Hamiltonian in a central force-field:

$$H = \underbrace{(C \cancel{\cdot} p - \beta mc^2)}_{H_0} - \frac{Ze^2}{r}$$

$$p = -i\hbar \text{ grad} \quad \therefore \underline{p}^* = -p$$

$$\beta^* = \beta \quad \alpha_x^* = \alpha_x \quad \alpha_y^* = -\alpha_y \quad \alpha_z^* = \alpha_z$$

$$\therefore H^* = C(-\alpha_x p_x + \alpha_y p_y - \alpha_z p_z) - \beta mc^2 - \frac{Ze^2}{r}$$

and $H^* \neq H$, by any means. However, we can put:

$$U = \gamma_y = \begin{pmatrix} 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \quad \text{to get} \quad UH^*U^{-1} = H$$

There will always exist such a matrix U whenever time is reversible in the problem. (and this will be true for most problems). However, there is no general way to construct U explicitly. This has to be done separately for each special case.

$$H\psi_a = E\psi_a \quad H^*\psi_a^* = E^*\psi_a^*$$

$$UH^*U^{-1} = H \quad \therefore H(U^+\psi_a^*) = E^*(U\psi_a^*)$$

We define the function ψ_{-a} by:

$$\psi_{-a}^* = U^+ C_a \psi_a \quad (C_a = \text{constant})$$

ψ_{-a} is the "reciprocal" eigenfunction. Clearly the unitary transformation U must work separately on H_0 and on V , therefore:

$UH_0^*U^{-1} = H_0$, also, and we can define a "reciprocal" base function ϕ_{-a} by:

$$\phi_{-a}^* = U^{-1} C_a \phi_a$$

ϕ_a will be an eigenfunction of H_0 belonging to energy E_0 , but not equal to ψ_a . For free particles without spin, the ϕ_a belonging to $\phi_a = e^{ikx \cdot I}$ is $\phi_{-a} = e^{-ik \cdot (-x)}$, i.e., the "reciprocal" wave is the wave in the opposite direction. In this particular case $C_a = 1$, but in general a constant $C_a \neq 1$ will be necessary. We first show that $|C_a|^2$ must be equal to 1 provided U is unitary (which we are free to do).

Proof:

$$1 = (\phi_{-a}, \phi_a) = (U C_a \phi_a^*, U C_a \phi_a^*) = \\ = |C_a|^2 (\phi_a^*, U^+ U \phi_a^*) = |C_a|^2 (\phi_a, (U^+ U)^* \phi_a) = 1$$

Now if U is unitary $(U^+ U)^* = 1$ and therefore $|C_a|^2 = 1$

Next we observe that there is one more restriction on the constants C_a :

$$\phi_a^* = U^+ \phi_a C_a \quad \phi_a = U C_{-a} \phi_{-a}^* \quad (?)$$

$$\text{Now clearly: } \phi_a = (\phi_a^*)^* = (U^{-1} C_a \phi_a)^* = (U^{-1})^* C_a^* U^{-1} \phi_a C_{-a}$$

$$\therefore \phi_a = C_a^* C_{-a} (U U^*)^{-1} \phi_a$$

We next observe that $U U^* = \lambda$, a multiple of the unit matrix, when operating upon ϕ_a . To show this we write

$$H_0 = (H_0^*)^* = (U H_0 U^{-1})^* = U^* H_0^* (U^{-1})^* = U^* U H_0 (U^* U)^{-1}$$

Therefore $U^* U$ commutes with H_0 , and we can pick our basis-functions ϕ_a so that they are eigenfunctions of $U^* U$ in addition to being eigenfunctions of H_0 . In the following we shall assume that such a choice has been made:

$$H_0 \phi_a = E_a \phi_a \quad (E_a \text{ real})$$

$$U^* U \phi_a = \lambda_a \phi_a$$

Then our previous condition:

$$U U^* \phi_a = C_a^* C_{-a} \phi_a = \lambda_a^* \phi_a$$

$$\text{becomes: } C_a^* C_{-a} = \lambda_a^+$$

In the example of the Dirac-hamiltonian:

$$U = \gamma_y \quad U^+ U = 1 \quad \text{But } U^+ = -\gamma_y, \text{ so } U^* U = -1$$

Therefore: $C_a^* C_{-a} = -1$ and we are not allowed to choose $C_a = 1$, all a

It must be remarked right here that all this discussion about C_a is not really essential to our result. The constants C_a will drop out in the final answer.

We now introduce the "time reversed" eigenfunctions.

$$(H_0 + V)\psi_a = E\psi_a \quad (H_0 + V)\psi_{-a}' = E^*\psi_{-a}'$$

The prime will be used to denote time reversed quantities. Following the same argument as before, we get:

$$\psi'_a = \phi_a + \frac{1}{E^* - E_0} V \psi'_a = \sum_b S'_{ba} \phi_a$$

$$S'_{ba} = S_{ba} + \frac{1}{E^* - E_0} (\phi_b, V \psi'_a) = S_{ba} + \frac{1}{E^* - E_0} T'_{ba}$$

This defines S'_{ba} and T'_{ba} . There will be a relation between T_{ba} and T'_{ba} . To find it we use the identity:

$$C_{-a} \psi_a = V \psi'_{-a}$$

Using the expansion $\psi_a = \sum_b \phi_b S_{ba}$ this gives:

$$C_{-a} \psi'_{-a} = \sum_b V \phi_b^* S_{-b,-a}^* = \sum_b \phi_b C_{-b} S_{-b,-a}^*$$

but we also have:

$$C_{-a} \psi'_{-a} = C_{-a} \sum_b \phi_b S'_{ba}$$

therefore we get the identity

$$C_{-a} S'_{ba} = C_{-b} S_{-b,-a}$$

From this it follows as an immediate algebraic consequence that:

$$C_{-a} T'_{ba} = T_{-b,-a}^* C_{-b}$$

This relates the transition $a \rightarrow b$ to the transition $(-a) \rightarrow (-b)$ and is essentially a reciprocity theorem but not the standard one (really it is half of the reciprocity theorem)

Variational Principle for the elements T_{ba} .

Consider the expression:

$$(\psi_b, V \psi_a) - (\psi_b, V \frac{1}{E - E_0} V \psi_a)$$

We first write this as:

$$(\psi_b, V \psi_a - \frac{1}{E - E_0} V \psi_a) = (\psi_b, V \phi_a) = (T_{ba})^*$$

We then write this as:

$$(\psi_b - \frac{1}{E^* - E_0} V \psi_b, V \psi_a) = (\phi_b, V \psi_a) = T_{ba}$$

This first of all provides the general proof of the reciprocity theorem:

$$(T_{ab})^* = T_{ba}$$

To show that this leads to the commonly known reciprocity theorem, we combine it with the result on the last section:

$$T'_{ab} = \frac{C_{-a}}{C_{-b}} T_{-a,-b}^* = T_{ba}^*$$

Taking the absolute square of both sides, and noting that:

$$|C_{-a}|^2 = |C_{-b}|^2 = 1$$

$$\text{We see that: } |T_{-a,-b}|^2 = |T_{ba}|^2$$

So the probability of the following two processes is equal:

I) $a \nearrow$ incident, scattering into b

II) $\xleftarrow{(-b)}$ incident, scattering into $\nearrow (-a)$

We now consider the expression:

$$\frac{1}{T_{ba}} = \frac{(\psi_b, V \psi_a) - (\psi_b, V \frac{1}{E - E_0} V \psi_a)}{(\psi_b, V \phi_a)(\phi_b, V \psi_a)} \quad (1)$$

It is independent of the normalization of ψ_b and ψ_a (a useful property) we further claim that this expression is stationary under variations of ψ_a and of ψ_b separately.

Proof:

$$\psi'_b \rightarrow \psi'_b + \delta \psi'_b$$

$$\frac{1}{T_{ba}} \rightarrow \frac{(\psi'_b + \delta \psi'_b, V \psi_a) - (\psi'_b + \delta \psi'_b, V \frac{1}{E - E_0} V \psi_a)}{(\psi'_b + \delta \psi'_b, V \phi_a)(\phi_b, V \psi_a)}$$

$$\frac{1}{T_{ba}} \rightarrow \frac{1}{(\psi_b, V \phi_a)(\phi_b, V \psi_a)} \left[1 - \frac{(\delta \psi'_b, V \phi_a)}{(\psi'_b, V \phi_a)} \right] \left[\text{Numerator} \right]$$

We pick out the coefficient of $\delta \psi'_b$, and set it = 0

$$(\delta \psi'_b, V \psi_a) - (\delta \psi'_b, V \frac{1}{E - E_0} V \psi_a) = 0$$

$$- [(\psi_b, V \psi_a) - (\psi_b, V \frac{1}{E - E_0} V \psi_a)] \frac{(\delta \psi'_b, V \phi_a)}{(\psi'_b, V \phi_a)} = 0$$

$$\therefore V \psi_a - V \frac{1}{E - E_0} V \psi_a = \frac{(\psi'_b, V \phi_a) - (\psi'_b, V \frac{1}{E - E_0} V \psi_a)}{(\psi'_b, V \phi_a)} V \phi_a$$

$$\psi_a = \left[\frac{(\psi'_b, V \phi_a) - (\psi'_b, V \frac{1}{E - E_0} V \psi_a)}{(\psi'_b, V \phi_a)} \right] \phi_a + \frac{1}{E - E_0} \psi_a$$

This is the correct expression for ψ_a , provided the bracket [] equals one, which it does. This proves that (1), the expression for $\frac{1}{T_{ba}}$ yields the correct equation for ψ_a if we put on the requirement that it be stationary under small variations of ψ'_b (2) Therefore, if we put in an approximately correct ψ'_b , the expression for $\frac{1}{T_{ba}}$ will be in error by the square of the error in ψ'_b .

A similar proof holds for variations of ψ_b . Here we see too, that we had to use ψ'_b rather than ψ_b in the formulation of

our variation principle, otherwise $\delta \psi_a = 0$ would have given an incorrect equation for ψ_b (this equation is however the correct one for ψ_b)

Use of the Variation Principle

If one does the usual Born approximation one solves the equation

$$\psi_a = \phi_a + \frac{1}{E - H_0} V \psi_a \text{ by iteration}$$

This leads to a power-series in the "perturbation" V . This power-series may or may not converge. (After all, power-series converge only within a limited circle of convergence). We can however substitute the approximation for ψ_a as obtained into our variation principle for ψ_a and replace by ϕ_a , this gives:

$$\frac{1}{T_{ba}} \approx \frac{(\phi_b, V \phi_a) - (\phi_b, V \frac{1}{E - H_0} V \phi_a)}{(\phi_b, \phi_a)^2}$$

We can take the reciprocal of this, T_{ba} , and expand the denominator to get

$$T_{ba} \approx (\phi_b, V \phi_a) - (\phi_b, V \frac{1}{E - H_0} V \phi_a) \quad (\text{Born})$$

But our expression for $\frac{1}{T_{ba}}$ is much better than that.

The Heitler Integral Equation

We again start with

$$\psi_a = \phi_a + \frac{1}{E - H_0} V \psi_a$$

$$\frac{1}{E - H_0} \rightarrow P\left(\frac{1}{E - H_0}\right) - i\pi \delta(E - H_0)$$

$$\psi_a - P\left(\frac{1}{E - H_0}\right)V \psi_a = \phi_a - i\pi \delta(E - H_0)V \psi_a$$

The expression on the righthand side is an eigenfunction of H_0 (not H) belonging to the eigenvalue E for:

$$\delta(E - H_0)V \psi_a = \delta(E - H_0) \sum_b \underbrace{\phi_b}_{T_{ba}} \underbrace{(\phi_b, V \psi_a)}_{(\sum_b (\phi_b) \phi_a) \phi_a} = \sum_b \delta(E - E_b) \phi_b T_{ba}$$

and in this sum only the terms with $E_b = E$ contribute.

We introduce the wave function χ_a by the equation:

$$\chi_a - P\left(\frac{1}{E - E_0}\right)V \psi_a = \phi_a$$

(χ_a is the incident wave modified by the inductive terms only) Then the correct solution of the whole problem is obtained by solving the pair of Hermitian integral equations:

$$\begin{aligned} \psi_a &= \chi_a - i\pi \sum_b \phi_b \delta(E - E_b) T_{ba} \\ \chi_a &= \phi_a + P\left(\frac{1}{E - H_0}\right)V \psi_a \end{aligned}$$

This pair is equivalent to the one original Non-Hermitian integral equation.

We are really interested, not in ψ_a itself but in $T_{ba} = (\phi_b, V \psi_a)$. We therefore introduce the quantities:

$$K_{ba} \equiv (\phi_b, V \phi_a) \quad (b, V \phi_b)$$

Then clearly

$$T_{ba} = K_{ba} - i\pi \sum_c K_{bc} \delta(E - E_c) T_{ca}$$

Now a run over all states "C" can be split into a integral over E_C with the weight function ρ_c (density states) and a sum (integral) over types C of states "C" with the same energy:

$$\sum_c \rightarrow \sum_c \int_c \rho_c dE_C$$

Then we get:

$$T_{ba} = K_{ba} - i\pi \sum_c \underbrace{K_{bc} \rho_c}_{\text{with } E_c = E} T_{ca}$$

Here b, a, c all belong to the same energy $E_a = E_b = E_c = E$. This is known as the Heitler integral equation.

To save writing we shall define matrix multiplication to mean $(AB)_{ab} = \sum_c A_{ac} B_{cb}$, a, b, c belong to the same energy. Observe that the unit matrix has elements δ_{ab}

Then the Heitler equation becomes:

$$T = K - i\pi K T$$

$$\text{with the formal solution: } T = \frac{K}{1 + i\pi K}$$

Theorem: K is hermitian.

Proof: Consider the expression:

$$(\chi_b, V \chi_a) - (\chi_b, V P\left(\frac{1}{E - H_0}\right)V \chi_a)$$

This expression can be written as:

$$(\chi_b, V [\chi_a - P\left(\frac{1}{E - H_0}\right)V \chi_a]) = (\chi_b, V \phi_a) = K_{ab}^*$$

or alternatively as:

$$\left(\chi_b - P\left(\frac{1}{E-H_0}\right) V \chi_b, V \chi_a \right) = (\phi_b, V \chi_a) = K_{ba}$$

Hermitian!

$$\therefore K_{ab}^* = K_{ba} \quad \text{or} \quad K \text{ is Hermitian.}$$

Theorem: The expression:

$$\frac{1}{K_{ba}} = \frac{(\chi_b, V \chi_a) - (\chi_b, V P\left(\frac{1}{E-H_0}\right) V \chi_a)}{(\chi_b, V \phi_a)(\phi_b, V \chi_a)}$$

is stationary under small variations of χ_b and χ_a separately.

Proof: Formally exactly the same as the previous proof for $\frac{1}{T_{ba}}$. We shall see later that K can be written as $K = -\frac{1}{\pi} \tan \delta$ so we have a variation principle for the cotangent of the phase shift δ .

The Scattering Matrix

We define the scattering matrix S by:

$$S = 1 - 2\pi i T = \frac{1 - \pi i K}{1 + \pi i K}$$

Clearly $S^+ = \frac{1 + \pi i K}{1 - \pi i K}$ and since we have just shown that K is hermitian, $S^+ = S^{-1}$, the scattering matrix is unitary (Remember that tick definition of multiplication used here). We put $K = -\frac{1}{\pi} \tan \delta$; since K is hermitian, no will be δ . Then:

$$S = \frac{1 + i \tan \delta}{1 - i \tan \delta} = \frac{\cos \delta + i \sin \delta}{\cos \delta - i \sin \delta} = e^{i\delta}$$

$$2\pi i T = 1 - S = 1 - e^{i\delta} = e^{i\delta} (e^{-i\delta} - e^{i\delta})$$

$$2\pi i T = -2i e^{i\delta} \sin \delta$$

$$\therefore T = -\frac{1}{\pi} e^{i\delta} \sin \delta$$

One usually diagonalizes the scattering matrix for scattering problems. This diagonalizes S , T and K at the same time, of course. In the simple problems with spherical symmetry, this means going to angular-momentum eigenfunctions (spherical harmonics).

The Fundamental Theorem of Optics

We use:

$$T = -\frac{1}{\pi} e^{i\delta} \sin \delta$$

$$\begin{aligned} -\pi T &= e^{i\delta} \sin \delta = \cos \delta \sin \delta + i \sin^2 \delta \\ +\pi T^+ &= -e^{-i\delta} \sin \delta = -\cos \delta \sin \delta + i \sin^2 \delta \\ \therefore -\pi(T - T^+) &= 2i \sin^2 \delta \end{aligned}$$

$$\text{On the other hand } T^+ T = \frac{1}{\pi^2} \sin^2 \delta$$

$$\text{Therefore: } T^+ T = -\frac{1}{\pi} \frac{T - T^+}{2i} = -\frac{1}{\pi} \Im T$$

Written out for the diagonal element (a, a) this becomes:

$$\sum_b |T_{ba}|^2 p_b = -\frac{1}{\pi} \Im (T_{aa})$$

The left side of this represents the total time rate of increase of probability away from state a . The right hand side is $-\frac{1}{\pi}$ times the imaginary part of the amplitude of the wave scattered in the forward direction.

Interpretation of S = unitary in terms of Conservation of Probability.

We introduce the energy explicitly as an index to our wave-functions ($\psi_{a,E}$ instead of ψ_a)

$$\psi_{a,E} = \phi_{a,E} + \sum_{E' \neq E} \frac{1}{E-E'} \phi_{b,E'} T_{b,E';a,E}$$

$$\text{No } \phi_{a,E} \text{ can be written as } \sum_{E' \neq E} \frac{S(E-E')}{E-E'} S_{ab} \phi_{b,E'}$$

Furthermore we remember that:

$$\left. \begin{aligned} \frac{1}{E-E'} &\rightarrow P\left(\frac{1}{E-E'}\right) - \pi i S(E-E') \\ \frac{1}{E^*-E'} &\rightarrow P\left(\frac{1}{E-E'}\right) + \pi i S(E-E') \end{aligned} \right\} \text{in the limit } S \gg 0$$

Therefore we can write:

$$S(E-E') = \frac{1}{2\pi i} \left[\frac{1}{E^*-E'} - \frac{1}{E-E'} \right]$$

$$\text{and: } \phi_{a,E} = \sum_{E' \neq E} \frac{1}{2\pi i} \frac{1}{p_a} \left[\frac{1}{E^*-E'} - \frac{1}{E-E'} \right] S_{ab} \phi_{b,E'}$$

This is a fancy way to saying that we can write the incident (plane) wave as a superposition of incoming ($\frac{1}{E^*-E'}$) and outgoing ($\frac{1}{E-E'}$) (spherical) wave.

The total wave function then becomes:

$$\begin{aligned} \psi_{a,E} &= \frac{1}{2\pi i} \sum_{E' \neq E} \sum_b \frac{1}{E^*-E'} \frac{S_{ab}}{p_a} \phi_{b,E'} - \\ &- \frac{1}{2\pi i} \sum_{E' \neq E} \sum_{E' \neq E} \frac{1}{E-E'} \left[\frac{S_{ab}}{p_a} - 2\pi i T_{b,E';a,E} \right] \phi_{b,E'} \end{aligned}$$

$$t_{a,E} = \frac{1}{2\pi i} \sum_{E',b} \left(\frac{1}{E^* - E'} T_{ab} \phi_{bE'} - \frac{1}{E - E'} S_{ab} \phi_{bE'} \right) \quad (?)$$

The ratio of the coefficients of the outgoing waves to that of the incoming wave is the scattering matrix, $S = e^{2i\delta}$, provided we restrict ourselves to states of the same energy as the incident wave.

We now look at the fundamental law of conservation of probability:

$$\frac{\partial}{\partial t} (t_{aE}, t_{bE'}) = 0$$

For $E \neq E'$, t_{aE} is orthogonal to $t_{bE'}$ and this is no restriction. So we assume $E = E'$ from the start. Now we substitute the expression on the last page for t_{aE} and a similar one for t_{bE} . We will use our trick definition of matrix multiplication again, by which $\frac{S_{ab}}{S_{ac}}$ is the (a,b) element of the unit matrix, and will be written as T_{ab} . We also observe that a time factor $e^{-\frac{i}{\hbar}Et}$ goes with the $\frac{1}{E-E'}$, a time factor $e^{-\frac{i}{\hbar}E''t}$ goes with the $\frac{1}{E'-E''}$. The scalar product $(t_{aE}, t_{bE'})$ will then have terms going as $e^{+i\frac{K}{\hbar}t}$, 1, and $e^{+i\frac{K}{\hbar}t}$. The time derivative will give a factor $-\frac{K}{\hbar}$, 0 respectively. Up to irrelevant factors we have then:

$$(t_{aE}, t_{bE'}) \propto \sum_c \frac{2\pi}{\gamma} \delta(E_0 - E') T_{ac} T_{cb} e^{-\frac{K}{\hbar}t} + \\ + \sum_c \frac{2\pi}{\gamma} \delta(E_0 - E') S_{ac}^* S_{cb} e^{+\frac{K}{\hbar}t} +$$

+ terms independent of time.

If we now require that the time-derivative of this be zero in the limit $\gamma \rightarrow 0$, we get:

$$\sum_c T_{ac} T_{cb} - \sum_c S_{ac}^* S_{cb} = 0 \\ (1)_{ab} - (S + S^*)_{ab} = 0$$

This completes the proof that the condition $S + S^* = 1$ is essentially a condition imposed by the requirement of conservation of probability.

The formal Theory of Scattering.

(Gell-Mann and Goldberger. Phys. Rev. 91, 398, 1953)

Derivation of the transition probability.

In a quantum-mechanical description of scattering, a system of two (or more) colliding parts is governed by a Hamiltonian H that includes interaction between them. We imagine that H is split into two parts, which we shall call K and V , such that if K were the entire Hamiltonian the colliding parts would have the same internal structure but would suffer no scattering.

We are interested in calculate the rate of transition from one such noninteracting state to another. The Schrödinger equation (with $\hbar=1$) for the system with interaction is:

$$i\partial_t \Psi(t) = (K+V) \Psi(t) \quad (1)$$

Let be $\Psi_i(t) = \phi_i e^{-iEt}$ the stationary state solutions (normalized to unity) of the Schrödinger equation in the absence of interaction.

$$i\partial_t \Psi_i(t) = K \Psi_i(t) \quad (2)$$

We shall consider the transition $\Psi_j \rightarrow \Psi_i$ caused by the interaction V . The "initial state" Ψ_j characterize the actual state Ψ_j of the real system. We may, knowing Ψ_j , find the rate of increase, during the time of scattering, of the probability that the real system is one of the "final states" Ψ_i .

Suppose that we examine the transition rates at times $t=0$. It is necessary to represent mathematically the way in which the state Ψ_j has been prepared during time $t < 0$, for example by directing an approximately collimated and monochromatic beam of particles at a scattering center. One might try a model in which, at some time T in the distant past, the system was in the "free" state Ψ_j , so that $\Psi_j(t) = e^{-iH(t-T)} \Psi_j(T)$. However, undesirable transients are introduced into the temporal dependence of Ψ_j by the somewhat unphysical assumption that the train of incident waves is released all at once at time T . Rather, one must represent the incident train as fed in over a period of time in the past, using a Ψ_j that is the a sum or average over T of the ones suggested above. For instance one could take $\Psi_j(t)$ as:

$$\frac{1}{2} \int_{-z}^0 dt e^{-iH(t-T)} \Psi_j(T)$$

with z allowed to approach $+\infty$ at the end of the calculation. We shall adopt the form that is most convenient mathematically; namely:

We are using the relation: $\Psi_j(t) = e^{-iHt} \Psi_j(0, T)$ where $T \rightarrow -\infty$. In order to define this limit we take:
 $\Psi_j(0, T \rightarrow -\infty) = \lim_{T \rightarrow -\infty} e^{iHT} \Psi_j(T)$ where $L \equiv \lim_{T \rightarrow -\infty} \int_0^T dTe^{iET}$ (see eq. (33))
 $\Psi_j^{(\epsilon)}(t) = \int_{-\infty}^0 dTe^{iET} e^{-iH(t-T)} \Psi_j(T) \quad (e^{iHT} \Psi_j(T) = e^{i(H-E)t} \phi_j)$

where $\epsilon \rightarrow 0$ in the evaluation of cross sections; but care must be exercised in passing to the limit since there is another limiting process to be performed. Our ϕ 's are normalized to unity in a large region of linear dimension L and volume L^3 . We must remember that z or its equivalent ϵ^{-1} , corresponding as it does to the length of the incident wave train divided by the group velocity v , may not exceed Lv^{-1} . When ϵ^{-1} and L both tend to infinity, quantities proportional to $\epsilon^{-1}L^{-3}$ will tend to zero.

The probability that the system is in state Ψ_i at time t is:

$$w_{ij}(t) = |\psi_{ij}(t)|^2 N_j^{-1} \quad (4)$$

where:

$$\psi_{ij}(t) = \langle \Psi_j(t) | \Psi_i(t) \rangle \quad (5)$$

and:

$$N_j = \langle \Psi_j(t) | \Psi_j(t) \rangle \quad (6)$$

(We have suppressed the index ϵ). The normalization N_j is independent of time because H is hermitian. ($i \partial_t \langle \Psi_j | \Psi_j \rangle = \langle \Psi_j | H^+ - H | \Psi_j \rangle = 0$)

From equation (3):

$$\Psi_j = e^{-iHt} \int_0^\infty dTe^{iET} e^{i(H-E_j)T} \phi_j$$

(since: $\Psi_j(T) = \phi_j e^{-iE_j T}$)

$$\therefore \Psi_j(t) = e^{-iHt} \underbrace{\frac{e}{\epsilon + i(H-E_j)}}_{\text{initial state}} \phi_j \quad (7)$$

But: $(H-E_j) \phi_j = V \phi_j$ "initial state" (time-independent) $\equiv \Psi_j(0)$

thus, for $t=0$: (in order to handle only the time independent part)

$$\Psi_j(0) = \frac{i \epsilon \phi_j}{E_j - H + i\epsilon} = \phi_j + \frac{(H-E_j) \phi_j}{E_j - H + i\epsilon}$$

$$\therefore \Psi_j(0) = \phi_j + \frac{1}{E_j - H + i\epsilon} V \phi_j \quad (8)$$

By algebraic manipulation:

$$\Psi_j(0) = \phi_j + \frac{1}{E_j - K + i\epsilon} V \Psi_j(0) \quad (9)$$

If V is to be treated as a small perturbation, by successive iterations we have:

$$\Psi_j(0) = \phi_j + \frac{1}{E_j - K + i\epsilon} V \phi_j + \frac{1}{E_j - K + i\epsilon} V \frac{1}{E_j - K + i\epsilon} V \phi_j + \dots$$

which connects (8) and (9). Using (9), we see that:

$$\psi_{ij}(0) = \delta_{ij} + \frac{1}{E_j - E_i + i\epsilon} R_{ij}(\epsilon) \quad (10)$$

where:

$$R_{ij}(\epsilon) = \langle \phi_i | V | \Psi_j(0) \rangle \quad (11)$$

The Green's function is:

$$G^{(+)}(E_j) = \lim_{\epsilon \rightarrow 0^+} \frac{1}{E_j - K + i\epsilon} \quad (12)$$

We will take it for granted from now on that:

$$\lim_{\epsilon \rightarrow 0^+} R_{ij}(\epsilon) L^3 \equiv R_{ij}$$

is free of singularities at $E_i = E_j$. From (5):

$$\psi_{ij} = \langle \phi_i | e^{i(E_i-H)t} | \Psi_j(0) \rangle = \psi_{ij}(t)$$

$$\therefore \psi_{ij}^{(n)}(0) = i^n \langle \phi_i | (E_i - H)^n | \Psi_j(0) \rangle$$

For the transition rate we need only:

$$\begin{aligned} \dot{\psi}_{ij}(0) &= i \langle \phi_i | E_i - H | \Psi_j(0) \rangle = -i \langle \phi_i | V | \Psi_j(0) \rangle \\ \therefore \dot{\psi}_{ij}(0) &= -i R_{ij}(\epsilon) \end{aligned} \quad (13)$$

From (10) and (13):

$$\begin{aligned} \left[\frac{d}{dt} |\psi_{ij}(t)|^2 \right]_{t=0} &= \left[\dot{\psi}_{ij}^*(t) \psi_{ij}(t) + \dot{\psi}_{ij}(t) \psi_{ij}^*(t) \right]_{t=0} = \\ &= \left\{ i R_{ij}^*(\epsilon) [\delta_{ij} + \frac{1}{E_j - E_i + i\epsilon} R_{ij}(\epsilon)] - \right. \\ &\quad \left. - i [\delta_{ij} + \frac{1}{E_j - E_i - i\epsilon} R_{ij}^*(\epsilon)] R_{ij}(\epsilon) \right\} = \\ \therefore \left[\frac{d}{dt} |\psi_{ij}(t)|^2 \right]_{t=0} &= 2 \delta_{ij} \operatorname{Im} R_{jj}(\epsilon) + \frac{2\epsilon}{(E_j - E_i)^2 + \epsilon^2} |R_{ij}(\epsilon)|^2 \end{aligned} \quad (14)$$

We consider now the normalization N_j of the state vector. Since ϕ_j are a complete set of states:

$$\sum_i |\psi_{ij}|^2 = N_j \quad (15)$$

Using (14) and (15), and the fact that N_j is constant in time, we see that:

$$2 \operatorname{Im} R_{jj}(\epsilon) + \sum_i \frac{2\epsilon}{(E_j - E_i)^2 + \epsilon^2} |R_{ij}(\epsilon)|^2 = 0 \quad (16)$$

Computing N_j from (10) and (15) we have:

$$N_j = 1 + \frac{2}{\epsilon} \operatorname{Im} R_{jj}(\epsilon) + \sum_i \frac{1}{(E_j - E_i)^2 + \epsilon^2} |R_{ij}(\epsilon)|^2 \quad (16)$$

With the use of (16) :

$$N_j = 1 + \frac{1}{\epsilon} \operatorname{Im} R_{jj}(\epsilon)$$

We may remark that $R_{jj}(\epsilon) \sim L^{-3}$ and thus the double limiting process makes $N_j \rightarrow 1$

Now the differential cross section for the transition $j \rightarrow i$ is equal to the transition rate divided by the flux $v L^{-3}$, where v is the relative velocity of the colliding systems. Except for the single state j , to be discussed afterward, we have for each i the following expression for the differential cross section, using (14):

$$\sigma_{ij} = \lim_{\substack{\epsilon \rightarrow 0^+ \\ L \rightarrow \infty}} \frac{2\epsilon}{(E_j - E_i)^2 + \epsilon^2} |R_{ij}(\epsilon)|^2 L^3 v^{-1} \quad (17)$$

$$\text{But: } \lim_{\epsilon \rightarrow 0} \frac{2\epsilon}{(E_j - E_i)^2 + \epsilon^2} = 2\pi \delta(E_j - E_i)$$

which is to be interpreted as 2π times the density in energy of final states i at energy E_j ; the conservation of energy is understood as well. (Cf. Heitler's book p. 139). If the volume in momentum space per unit energy about state i is w_i , then the density of final states is $L^3 w_i$ and we have:

$$\sigma_{ij} = 2\pi |R_{ij}|^2 w_i v^{-1} \quad (18)$$

It is clear that the single state j considered as a possible final state will contribute nothing to the density of final states; nevertheless, the rate of change of w_{jj} is of importance when considered as the rate of depletion of the initial state. From the fact that the normalization is preserved in time it is clear that the rate of decrease of w_{jj} is given precisely by the rate of transition into all other states $i \neq j$. If we set $i=j$ in eq. (14) we obtain:

$$N_j \frac{d}{dt} w_{jj} \Big|_{t=0} = 2 \operatorname{Im} R_{jj}(\epsilon) + \frac{2}{\epsilon} |R_{jj}(\epsilon)|^2$$

In the limit $L \rightarrow \infty$ (and $\epsilon \rightarrow 0^+$) the second term is vanishingly small

$$\therefore -2 \operatorname{Im} \frac{R_{jj}}{L^3} = \frac{1}{L^3} \sum_{i \neq j} \frac{2\pi}{L^3} |R_{ij}|^2 \delta(E_j - E_i)$$

or:

$$\sum_{i \neq j} \sigma_{ij} = -\frac{2}{v} \operatorname{Im} R_{jj} \quad (19)$$

the well-known optical theorem.

From the preceding discussion it has become clear that for practical purposes one may ignore the complications of the double limiting processes

and deal with the state vector $\psi_j^{(+)}$ obtained by letting $\epsilon \rightarrow 0$, which evidently satisfies:

$$\psi_j^{(+)} = \phi_j + G^{(+)}(E_j) V \psi_j^{(+)} \quad (20)$$

Cross sections can be computed from the quantities:

$$R_{ij} = \langle \phi_i | V | \psi_j^{(+)} \rangle \quad R_{ij} \equiv \langle \phi_i | R | \phi_j \rangle = \langle \phi_i | V | \psi_j^{(+)} \rangle \quad (21)$$

in an obvious way. It is evident from (9) that $\psi_j^{(+)}$ is an eigenstate of the total Hamiltonian with eigenvalue E_j . It is the conventional stationary solution of the scattering problem corresponding to an "incoming wave" ϕ_j .

Although it is useful to work with $\psi_j^{(+)}$, it is necessary to exercise care on account of its singular character when expressed in terms of ϕ 's. For example, the operator K is not Hermitian when it appears between ϕ_j and $\psi_j^{(+)}$, since they satisfy different boundary conditions at infinity. Rather:

$$\langle K \phi_j | \psi_j^{(+)} \rangle - \langle \phi_j | K \psi_j^{(+)} \rangle = \langle \phi_j | V | \psi_j^{(+)} \rangle$$

For most purposes it is safe to consider the normalization

$$\langle \psi_j^{(+)} | \psi_j^{(+)} \rangle = 1$$

S matrix formalism

We shall outline the connection between the preceding discussion and the formalism of the interaction representation. Starting with the Schrödinger equation (1) we remove, in the usual way, the time dependence of the state vector associated with K by a unitary transformation to the interaction representation. Let

$$\Psi'(t) = e^{iKt} \Psi(t) \quad (21)$$

According to our definition, the interaction representation reduces to the Schrödinger representation at $t=0$. The new state vector satisfies:

$$i\partial_t \Psi'(t) = V(t) \Psi'(t) \quad (22)$$

where: $V(t) = e^{iKt} V e^{-iKt}$ (23)

We introduce the unitary operator $U(t, t_0)$ such that:

$$\Psi'(t) = U(t, t_0) \Psi'(t_0) \quad (24)$$

for each solution $\Psi'(t)$ of (22). $U(t, t_0)$ has two obvious properties:

$$\left. \begin{aligned} U(t, t) &= 1 \\ U(t, t_0) &= U(t, t') U(t', t_0) \end{aligned} \right\} \quad (25)$$

Since:

$$\Psi(t) = e^{-iH(t-t_0)} \Psi(t_0)$$

from (21) & (24) we have:

$$U(t, t_0) = e^{iKt} e^{-i(K+V)(t-t_0)} e^{-iKt_0} \quad (26)$$

To express $U(t, t_0)$ in terms of quantities in the interaction representation, we differentiate (26) with respect to t :

$$i\partial_t U(t, t_0) = e^{iKt} V e^{-i(K+V)(t-t_0)} e^{-iKt_0}$$

which we may rewrite, using (23) and (26), as:

$$i\partial_t U(t, t_0) = V(t) U(t, t_0) \quad (27)$$

Integrating we have:

$$U(t, t_0) = 1 - i \int_{t_0}^t dt' V(t') U(t', t_0) \quad (28)$$

If we differentiate (26) with respect to t_0 and then integrate, we obtain

$$U(t, t_0) = 1 + i \int_t^{t_0} dt' U(t, t') V(t') \quad (29)$$

The formal solutions of (28) and (29) by iteration can be written, with the aid of Dyson's ordering operation, (Cf. Dyson, Phys. Rev. 75, 486, 1949) as:

$$U(t, t_0) = \left(\exp \left[-i \int_{t_0}^t dt' V(t') \right] \right)_+ \quad (30)$$

and:

$$U(t, t_0) = \left(\exp \left[i \int_t^{t_0} dt' V(t') \right] \right)_- \quad (31)$$

respectively, where the symbol $(_)_+$ means that the terms in the power series development are to be ordered with the functions of earliest times standing to the right and $(_)_-$ indicates ordering in the opposite sense.

It is customary to introduce operators such as $U(t, -\infty)$ by allowing t_0 to approach $-\infty$ in such equations as (28)-(31). That it is not completely straightforward to do so becomes clear if we try to substitute $t_0 = -\infty$ into eq. (26). However, we are faced with no great mystery. The integrals in (28)-(31) may be exemplified by the second term in the expansion of (30):

$$-i \int_{t_0}^t dt' V(t') = -i \int_{t_0}^t dt' e^{iKt'} V e^{-iKt'} \quad (TBA)$$

The limit as t_0 tends to $-\infty$ of a matrix element of this operator will exist only if the limit is defined in such a way that oscillatory terms are made to vanish at $-\infty$. But with respect to such a limiting process, the limit of eq. (26) will have meaning as well, as we shall see. Moreover, the work of the preceding section has already provided us with a suitable limiting process.

Let us transform the state vector $\Psi_j^{(\epsilon)}(t)$ to the interaction representation using (21):

$$\Psi_j^{(\epsilon)}(t) = e^{iKt} e^{-iHt} \lim_{\epsilon \rightarrow 0^-} \int_0^\infty dT e^{\epsilon T} e^{iHT} e^{-iKT} \phi_j \quad (32)$$

which we may write, using (26), as:

$$\Psi_j^{(\epsilon)}(t) = \lim_{\epsilon \rightarrow 0^-} \int_0^\infty dT e^{\epsilon T} U(t, T) \phi_j \quad (33)$$

Now:

$$L f(T) \equiv \lim_{T \rightarrow -\infty} \lim_{\epsilon \rightarrow 0^+} \int_0^\infty dT e^{\epsilon T} f(T)$$

is an example of the kind of limiting process we need. If f possesses a genuine limit as $T \rightarrow -\infty$, the L operation yields the same one; but if f oscillates as $T \rightarrow -\infty$ the L operation gives 0. So we will take:

$$U(t, -\infty) = \lim_{\epsilon \rightarrow 0^+} \int_0^\infty dT e^{\epsilon T} U(t, T) \quad (34)$$

In an analogous way, we define:

$$U(\infty, t) = \lim_{\epsilon \rightarrow 0^+} \int_0^\infty dT e^{-\epsilon T} U(T, t) \quad (35)$$

etc. All the relations are now true that can be obtained by setting t or t_0 equal to $\pm \infty$ as in the integral equation of the interaction representation. One may show, for example, that eq. (28) has the limiting form:

$$U(t, -\infty) = 1 - i \int_{-\infty}^t dt' V(t') U(t', -\infty)$$

The Heisenberg's S matrix is then:

$$S \equiv U(\infty, -\infty) = 1 - i \int_{-\infty}^\infty dt' V(t') U(t', -\infty) \quad (36)$$

Now, from (34) and (26) we have:

$$U(t, -\infty) = e^{iKt} e^{-iHt} \lim_{\epsilon \rightarrow 0^+} \int_0^\infty dT e^{\epsilon T} e^{iHT} e^{-iKT}$$

Using the completeness relation:

$$1 = \sum_j \phi_j \rangle \langle \phi_j$$

we find:

$$U(t, -\infty) = e^{iKt} e^{-iHt} \lim_{\epsilon \rightarrow 0^+} \sum_j \int_0^\infty dT e^{\epsilon T} e^{iHT} e^{-iE_j T} \phi_j \rangle \langle \phi_j = \\ = e^{iKt} e^{-iHt} \lim_{\epsilon \rightarrow 0^+} \sum_j \frac{\epsilon}{\epsilon + i(H - E_j)} \phi_j \rangle \langle \phi_j \quad (36')$$

and (20)

In view of (7) we have:

$$U(0, -\infty) = \sum_j +_j^{(+)} \times \phi_j \quad (37)$$

$$\text{or: } U(0, -\infty) \phi_j = +_j^{(+)} \quad (38)$$

The operator $U(0, -\infty) \equiv \Omega^{(+)}$, is clearly the one that forms the singular wave-function matrix of Möller:

$$\langle \phi_i | \Omega^{(+)} | \phi_j \rangle = \langle \phi_i | +_j^{(+)} \rangle \quad (38')$$

Acting on the state ϕ_j , it produces that eigenstate of the total Hamiltonian, corresponding to ϕ_j as an incident wave. Similarly the operator

$$U(0, +\infty) \equiv \Omega^{(-)} \quad (39)$$

(here we need: $U(t, +\infty) = \lim_{\epsilon \rightarrow 0^+} \int_0^\infty d\tau e^{-\epsilon\tau} U(t, \tau)$)

instead of (34) carries ϕ_j into the eigenstate of the total Hamiltonian corresponding to ϕ_j as an outgoing wave:

$$\Omega^{(-)} \phi_j = +_j^{(-)} = \lim_{\epsilon \rightarrow 0^+} \frac{\epsilon}{\epsilon - i(H - E_j)} \phi_j$$

Instead of (20), we have for $+_j^{(-)}$ the equation:

$$+_j^{(-)} = \phi_j + G^{(-)}(E_j) V +_j^{(-)} \quad (40)$$

where $G^{(-)}(E_j) = \lim_{\epsilon \rightarrow 0^+} \frac{1}{E_j - K - i\epsilon} \quad (41)$

Let us now establish the properties of U matrices with infinite arguments corresponding to eq. (25) for finite times. It can easily be seen from (26) and (35) that:

$$U(\infty, t) = U(\infty, 0) U(0, t) \quad (42)$$

and by (34): $U(\infty, -\infty) = U(\infty, 0) U(0, -\infty) \quad (42)$

Now: $U(\infty, -\infty) = S$ and $U(0, -\infty) = \Omega^{(+)}$ but $U(\infty, 0)$ remains to be discussed. From (25):

$$U(t, t_0) U(t_0, t) = U(t_0, t) U(t, t_0) = 1$$

Since the U 's are unitary for finite times we have:

$$U(t, t_0) = U(t_0, t)$$

If we apply (34) or (35) to this equation, it remains unchanged and thus:

$$U(\pm \infty, 0) = U(0, \pm \infty)^+ \quad (43)$$

and (42) is:

$$S = \Omega^{(-)} + \Omega^{(+)} \quad (44)$$

Using the equations (37) and (43), and the completeness of the ϕ 's we have:

$$\begin{aligned} U(-\infty, 0) U(0, -\infty) &= \Omega^{(+)} + \Omega^{(+)} = \sum_{i,j} \phi_i \langle +_i^{(+)} | +_j^{(+)} \rangle \langle \phi_j = \\ &= \sum_i \phi_i \langle \phi_i \rangle = 1 \end{aligned}$$

with the use of the limiting normalization to unity of the $+_j^{(+)}$. Similarly:

$$U(\infty, 0) U(0, \infty) = \Omega^{(-)} + \Omega^{(-)} = 1$$

However the Ω 's are not necessarily unitary, since:

$$\Omega^{(\pm)} \Omega^{(\pm)} = \sum_i +_i^{(\pm)} \times +_i^{(\pm)} \quad (45)$$

is not necessarily 1. If there are bound states among the eigenstates of H , that is, states of energy less than that of any eigenstate of K with the same symmetry quantum numbers, then the $\Omega^{(\pm)}$ are not a complete set, and (45) may be restated as:

$$\Omega^{(\pm)} \Omega^{(\pm)} = 1 - \sum_\alpha +_\alpha \langle +_\alpha \rangle$$

where the $+_\alpha$ are the bound states, satisfying:

$$H +_\alpha = E_\alpha +_\alpha$$

In order to verify directly what is implicit in the preceding equations, namely:

$$\Omega^{(\pm)} + +_\alpha = 0 \quad (46)$$

as well as that: $\Omega^{(\pm)} + +_\alpha^{(\pm)} = \phi_i$

let us use (32), (34) and (35) which yield:

$$\Omega^{(\pm)} + + = \lim_{\epsilon \rightarrow 0^+} \frac{\epsilon}{\epsilon \pm i(K-E)} +$$

where $+$ is any eigenfunction of H with eigenvalue E . For a bound state $\Omega^{(\pm)}$ $K-E$ can never vanish, since K has no eigenvalues as low as E ; hence the relation (46). For a state in the continuum, we have:

$$\lim_{\epsilon \rightarrow 0^+} \frac{\epsilon}{\epsilon \pm i(K-E)} +^{(\pm)} = [1 - G^{(\pm)}(E)V] +^{(\pm)} = \phi$$

by (39) and (40); hence the relation (47).

The matrix elements of the S matrix may be computed as follows: from (36') and (37):

$$U(t, -\infty) = e^{iKt} \sum_j e^{-i\varepsilon_j t} \psi_j^{(+)} \rangle \langle \phi_j$$

and so:

$$V(t)U(t, -\infty) = \sum_{ij} \phi_i \rangle \langle \phi_i | e^{i(\varepsilon_i - \varepsilon_j)t} V \psi_j^{(+)} \rangle \langle \phi_j$$

Substituting in (36):

$$S = 1 - \sum_{ij} \phi_i \rangle \langle \phi_i | 2\pi i \delta(\varepsilon_i - \varepsilon_j) R_{ij} \langle \phi_j$$

or:

$$S_{ij} = \langle \phi_i | S | \phi_j \rangle = \delta_{ij} - 2\pi i \delta(\varepsilon_i - \varepsilon_j) R_{ij} \quad (48)$$

Another interesting form is provided by substituting (44) into the definition of S_{ij} :

$$\begin{aligned} S_{ij} &= \langle \phi_i | \mathcal{L}^{(-)} + \mathcal{L}^{(+)} | \phi_j \rangle = \\ &= \langle \mathcal{L}^{(-)} \phi_i | \mathcal{L}^{(+)} \phi_j \rangle = \langle \psi_i^{(-)} | \psi_j^{(+)} \rangle \end{aligned} \quad (49)$$

We show now that S is unitary. This may be done in a variety of ways. From equations (44) and (45) we have:

$$\begin{aligned} S^* S &= \mathcal{L}^{(+)} + \mathcal{L}^{(-)} \mathcal{L}^{(-)} + \mathcal{L}^{(+)} = \\ &= \mathcal{L}^{(+)} + [1 - \sum_k \psi_k \rangle \langle \psi_k] \mathcal{L}^{(+)} = 1 - \mathcal{L}^{(+)} + \sum_k \psi_k \rangle \langle \psi_k \mathcal{L}^{(+)} \end{aligned}$$

The second term is zero, since $\mathcal{L}^{(+)}$ operating on a state ψ_j produces a state $\psi_j^{(+)}$ [according to eq. (38')] which is orthogonal to the bound states ψ_k . Then:

$$S^* S = 1$$

The remainder is as follows:

$$\begin{aligned} S S^* &= \mathcal{L}^{(-)} \mathcal{L}^{(+)} \mathcal{L}^{(+)} + \mathcal{L}^{(-)} = \\ &= 1 - \mathcal{L}^{(+)} + \sum_k \psi_k \rangle \langle \psi_k \mathcal{L}^{(-)} = 1 \end{aligned}$$

since $\mathcal{L}^{(-)}$ produces a state $\psi^{(-)}$ which is orthogonal to the ψ_k .

Examples.

We consider now scattering processes in which there are two potentials acting: V and U . We want treat one of this exactly and the other approximately. At first sight all might appear to be trivial: one would replace the states

ϕ by the states ψ which are eigenfunctions of $K+U$, where U is the part to be treated exactly. The cross section can be obtained of the expression:

$$\langle \psi | V | \psi^{(+)} \rangle$$

Let us see to what extent such a procedure is legitimate. The difficulty arises from the fact that the cross section for the process are classified in terms of truly non-interacting final states. The true state vector is defined by:

$$\psi_a^{(+)} = \phi_a + \frac{1}{E - K + i\epsilon} (U + V) \phi_a^{(+)} \quad (50)$$

where ϕ_a is an eigenstate of K belonging to energy E . (The common energy of initial and final states will be called E). The probability of transition to another plane wave state ϕ_b is proportional to the absolute square of

$$R_{ba} = \langle \phi_b | R | \phi_a \rangle = \langle \phi_b | U + V | \psi_a^{(+)} \rangle \quad (51)$$

This is clearly the quantity of physical interest, the transition rate into a true plane wave state ϕ_b . We shall see that eq. (51) can indeed be written in the form $\langle \psi | V | \psi^{(+)} \rangle$, but only with a suitable choice of boundary conditions on ψ . Let us introduce the state vectors $\psi_b^{(-)}$ analogous to the $\psi_a^{(-)}$ used previously:

$$\psi_b^{(-)} = \phi_b + \frac{1}{E - K - i\epsilon} U \phi_b^{(-)} = \phi_b + \frac{1}{E - K - U} U \phi_b$$

$$\therefore \phi_b = [1 - \frac{1}{E - K - i\epsilon} U] \psi_b^{(-)}$$

Substituting in (51) and using (50) we have:

$$R_{ba} = \langle \psi_b^{(-)} | (1 - U \frac{1}{E - K + i\epsilon}) (U + V) | \psi_a^{(+)} \rangle =$$

$$= \langle \psi_b^{(-)} | U + V - U \frac{1}{E - K + i\epsilon} (U + V) | \psi_a^{(+)} \rangle =$$

$$= \langle \psi_b^{(-)} | U + V | \psi_a^{(+)} \rangle - \langle \psi_b^{(-)} | U | \psi_a^{(+)} \rangle - \langle \psi_b^{(-)} | V | \psi_a^{(+)} \rangle$$

$$\therefore R_{ba} = \langle \psi_b^{(-)} | V | \psi_a^{(+)} \rangle + \langle \psi_b^{(-)} | U | \phi_a \rangle \quad (52)$$

It is very easy to show that: (Cf. Lippmann-Schwinger paper eq. (63))

$$\langle \psi_b^{(-)} | U | \phi_a \rangle = \langle \phi_b | U | \psi_a^{(+)} \rangle$$

$$\text{where: } \psi_a^{(+)} = \phi_a + \frac{1}{E - K + i\epsilon} U \phi_a^{(+)} \quad (53)$$

The second term in (52) is simply the scattering amplitude which $\langle \psi_b^{(-)} | U | \phi_a \rangle = \langle \phi_b | U | \phi_a \rangle + \langle \phi_b | U \frac{1}{E - K + i\epsilon} U | \phi_a \rangle = \langle \phi_b | U | \psi_a^{(+)} \rangle$

$$\text{so: } R_{ba} \equiv \langle \phi_b | U + V | \psi_a^{(+)} \rangle = \langle \phi_b | U | \psi_a^{(+)} \rangle + \langle \psi_b^{(-)} | V | \psi_a^{(+)} \rangle \\ \simeq \langle \phi_b | U | \psi_a^{(+)} \rangle + \langle \psi_b^{(-)} | V | \psi_a^{(+)} \rangle$$

would be found even if $V=0$. The implicit dependence of $\psi_a^{(+)}$ on U may be seen by remarking that $\psi_a^{(+)}$ also satisfies:

$$\psi_a^{(+)} = \psi_a^{(+)} + \frac{1}{E - K - U + i\epsilon} V \psi_a^{(+)} \quad (54)$$

which we can derive directly.

From (50) it follows:

$$\psi_a^{(+)} = \phi_a + \frac{1}{E - K - U - V + i\epsilon} (U + V) \phi_a \quad (55)$$

and from (53):

$$\psi_a^{(+)} = \phi_a + \frac{1}{E - K - U + i\epsilon} U \phi_a \quad (56)$$

Subtracting this equations we have:

$$\begin{aligned} \psi_a^{(+)} - \psi_a^{(+)} &= \frac{1}{E - K - U - V + i\epsilon} [V + V - \frac{E - K - U - V + i\epsilon}{E - K - U + i\epsilon} V] \phi_a = \\ &= \frac{1}{E - K - U - V + i\epsilon} V [1 + \frac{1}{E - K - U + i\epsilon} V] \phi_a \end{aligned}$$

and from eq.(56) again:

$$\psi_a^{(+)} = \psi_a^{(+)} + \frac{1}{E - K - U - V + i\epsilon} V \psi_a^{(+)}$$

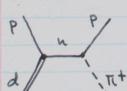
which is solution of (54). If V is small, eq.(52) is approximately:

$$R_{ba} \simeq \langle \psi_b^{(-)} | V | \psi_a^{(+)} \rangle + \langle \phi_b | U | \psi_a^{(+)} \rangle \quad (57)$$

This expression takes the potential U into account exactly as long as one is content with first order accuracy in V . It is to be noticed that to second order there is an additional U dependence since:

$$\psi_a^{(+)} = \psi_a^{(+)} + \frac{1}{E - K - U + i\epsilon} V \psi_a^{(+)} + \dots$$

In the case of the photoelectric effect or the process $\pi^+ + d \rightarrow 2p$ one is confronted with a slightly new problem. One is dealing with an initial state which although it lies in the continuum, is essentially a bound state. We shall keep in mind, for the sake of terminology, the process $\pi^+ + d \rightarrow 2p$. The physics of the problem leads us to the state vector $\Psi_a^{(\epsilon)}$ defined by:



$$\Psi_a^{(\epsilon)} = \psi_0 + \frac{1}{E_a - K + i\epsilon} V \psi_a^{(\epsilon)} \quad (\text{cf. eq. (54)}) \quad (58)$$

where ψ_0 represents the product of a plane wave meson state vector and a bound deuteron state vector. ψ_0 satisfies the integral equation:

$$\psi_0 = \frac{1}{E_a - K + i\epsilon} U \psi_0 \quad (\text{i.e. } (K + U) \psi_0 = E_a \psi_0) \quad (58')$$

where U is the deuteron potential. The meson coordinates are contained

in a completely trivial way in this equation since there is no interaction. It is convenient however, not to make an explicit separation. We now ask for the rate of transition into a plane wave state in the usual way: $i\omega_{ba} = N_a^{-1} \frac{\partial}{\partial t} |\langle \phi_b | \Psi_a \rangle|^2$

$$N_a \dot{w}_{ba} = \frac{\partial}{\partial t} |\langle \phi_b | e^{i(E_b - K - U - V)t} | \Psi_a^{(\epsilon)} \rangle|^2 \quad (59)$$

(We must, of course, keep ϵ finite in order that the necessary partial integrations can be carried out.) We shall evaluate (59) at $t=0$. In a similar way that a previous calculation we obtain:

$$N_a \dot{w}_{ba} = -i \langle \phi_b | U + V | \Psi_a^{(\epsilon)} \rangle \langle \phi_b | \Psi_a^{(\epsilon)} \rangle^* + \text{c.c.}$$

The evaluation of $\langle \phi_b | \Psi_a^{(\epsilon)} \rangle$ proceeds as follows: First write $\Psi_a^{(\epsilon)}$ in the form:

$$\Psi_a^{(\epsilon)} = \psi_0 + \frac{1}{E_a - K - U - V + i\epsilon} V \psi_0$$

$$\begin{aligned} \text{Then: } \langle \phi_b | \Psi_a^{(\epsilon)} \rangle &= \langle \phi_b | \psi_0 \rangle + \langle \phi_b | \frac{1}{E_a - K - U - V + i\epsilon} V | \psi_0 \rangle = \\ &= \langle \phi_b | \psi_0 \rangle + \langle \phi_b | \frac{1}{E_a - K + i\epsilon} V | \psi_0 \rangle + \\ &\quad + \langle \phi_b | \frac{1}{E_a - K + i\epsilon} (U + V) \frac{1}{E_a - K - U + i\epsilon} V | \psi_0 \rangle \\ &= \langle \phi_b | \psi_0 \rangle + \langle \phi_b | \frac{1}{E_a - K + i\epsilon} V | \psi_0 \rangle + \\ &\quad + \langle \phi_b | \frac{1}{E_a - K + i\epsilon} (U + V) | \Psi_a^{(\epsilon)} - \psi_0 \rangle = \\ &= \langle \phi_b | \psi_0 - \frac{1}{E_a - K + i\epsilon} U \psi_0 \rangle + \langle \phi_b | \frac{1}{E_a - K + i\epsilon} (U + V) | \Psi_a^{(\epsilon)} \rangle \end{aligned}$$

From (58') the first term is zero and then:

$$\langle \phi_b | \Psi_a^{(\epsilon)} \rangle = \frac{1}{E_a - E_b + i\epsilon} \langle \phi_b | U + V | \Psi_a^{(\epsilon)} \rangle$$

Proceeding in the now familiar way we deduce:

$$\begin{aligned} N_a \dot{w}_{ba} &= -\frac{i}{E_a - E_b - i\epsilon} |\langle \phi_b | U + V | \Psi_a^{(\epsilon)} \rangle|^2 + \text{c.c.} = \\ &= \frac{2\epsilon}{(E_a - E_b)^2 + \epsilon^2} |\langle \phi_b | U + V | \Psi_a^{(\epsilon)} \rangle|^2 \end{aligned}$$

In the limit $\epsilon \rightarrow 0^+$ we have:

$$\begin{aligned} \frac{2\epsilon}{(E_a - E_b)^2 + \epsilon^2} &\rightarrow 2\pi \delta(E_a - E_b) \\ N_a &\rightarrow 1 \quad \Psi_a^{(\epsilon)} \rightarrow \psi_a^{(+)} \end{aligned}$$

$$\therefore \nu_{ba} = 2\pi |\langle \phi_b | V + V^\dagger | \psi_a^{(+)} \rangle|^2 \delta(E_a - E_b) \quad (60)$$

Now we shall transcribe this ~~standard~~ matrix element in a manner similar to that used in connection with (51). This time, however, we substitute for ψ_b from the equation:

$$\psi_b^{(-)} = \phi_b + \frac{1}{E - K - V - i\epsilon} V \phi_b$$

The common energy of ϕ_b and $\psi_a^{(+)}$ is again denoted by E . We write:

$$\begin{aligned} \nu_{ba} &= \langle \phi_b | V + V^\dagger | \psi_a^{(+)} \rangle = \\ &= \langle \phi_b | V | \psi_a^{(+)} \rangle + \langle \psi_b^{(-)} | V | \psi_a^{(+)} \rangle - \langle \frac{1}{E - K - V - i\epsilon} V \phi_b | V | \psi_a^{(+)} \rangle \\ &= \langle \phi_b | V | \psi_a^{(+)} \rangle + \langle \psi_b^{(-)} | V | \psi_a^{(+)} \rangle - \langle \phi_b | V \frac{1}{E - K - V + i\epsilon} V | \psi_a^{(+)} \rangle = \\ &= \langle \phi_b | V | \psi_a^{(+)} \rangle + \langle \psi_b^{(-)} | V | \psi_a^{(+)} \rangle - \langle \phi_b | V | \psi_a^{(+)} - \psi_0 \rangle. \end{aligned}$$

$$\text{Finally: } \nu_{ba} = \langle \psi_b^{(-)} | V | \psi_a^{(+)} \rangle + \langle \phi_b | V | \psi_0 \rangle \quad (61)$$

In the class of examples being considered, where ψ_0 is the product of a plane wave state and a bound state, the second term vanishes. Hence the transition probability per unit time becomes:

$$\nu_{ba} = 2\pi |\langle \psi_b^{(-)} | V | \psi_a^{(+)} \rangle|^2 \delta(E_a - E_b) \quad (62)$$

It is perhaps worth noting that eq. (62) as well as the analogous one for an initial continuum, contained in (52), would not be correct with $\psi_b^{(+)}$ written in place of $\psi_b^{(-)}$.

Time-dependent Perturbation Theory.

P.A.M. Dirac Proc. Roy. Soc. A 112, 661 (1926)
L. Schiff. Quantum Mechanics p. 189 (1949)

Let us consider a system whose Hamiltonian can be written as:

$$H = K + V$$

We assume that:

- 1) We know the solutions for the part K (unperturbed Hamiltonian)
- 2) V is small.

We want construct solutions of the equation:

$$i\partial_t \Psi = H\Psi \quad (1)$$

in terms of the solutions of the equation

$$i\partial_t \Phi = K\Psi \quad (2)$$

Before to start this problem, let us study a little the equation (2). The general ~~exp~~ solution of this eq. can be written as:

$$\Phi = \sum_j c_j \Phi_j \quad (3)$$

where the Φ_j 's form a complete orthonormal set of functions, i.e.

$$(\Phi_j, \Phi_k) = \delta_{jk} \quad (4)$$

The explicit form of this functions is:

$$\Phi_j = \phi_j e^{-iE_j t}$$

where the time-independent functions ϕ_j satisfy the equation:

$$K\phi_j = E_j \phi_j \quad (5)$$

From (4) it follows: $(\phi_j, \phi_k) = \delta_{jk}$

The physical meaning of the coefficients c_j in the expansion (3) is that the expression $|c_j|^2$

represents the probability of finding the system in the state j . In order to maintain consistent this interpretation, we normalize the Φ functions to unity, i.e.: $(\Phi, \Phi) = \sum_j |c_j|^2 = 1$

We are now in position to tackle our problem. We expand the functions

Ψ in terms of the Φ 's:

$$\Psi = \sum_j a_j(t) \Phi_j$$

where now the coefficients evidently depend on the time. Explicitly we have:

$$\Psi(t) = \sum_j a_j(t) \Phi_j e^{-iE_j t}$$

Substitution of this expansion in equation (1) gives: (using also eq. (5))

$$i \sum_j \dot{a}_j \Phi_j e^{-iE_j t} = \sum_j a_j V \Phi_j e^{-iE_j t}$$

Multiplying both members for Φ_k and integrating we have:

$$\dot{a}_k = -i \sum_j a_j V_{kj} e^{i\omega_{kj} t} \quad (6)$$

where: $V_{kj} \equiv (\Phi_k, V \Phi_j)$ and $\omega_{kj} \equiv E_k - E_j$

The group of equations (6) is exactly equivalent to the equation (1). The physical meaning of the amplitudes a_m , as follows from the preceding discussion is that $|a_j(t)|^2$

is the probability of finding the system in the state j at time t . It may be chosen in such way that:

$$a_j(t \rightarrow -\infty) = c_j \quad (7)$$

The total probability:

$$(\Psi, \Psi) = \sum_j |a_j(t)|^2$$

is constant in time as a consequence of the Hermiticity of H . But it can be proved directly using the equations (6):

$$\begin{aligned} \frac{d}{dt} (\Psi, \Psi) &= \sum_j \frac{d}{dt} |a_j|^2 = \sum_j (\dot{a}_j^* a_j + a_j^* \dot{a}_j) = \\ &= i \sum_{jk} [a_j a_k^* V_{kj} e^{i\omega_{kj} t} - a_k a_j^* V_{jk} e^{i\omega_{jk} t}] = 0 \end{aligned}$$

From (7) it follows that we can choose:

$$(\Psi, \Psi) = 1$$

The perturbation approximation consists in replacing $V \rightarrow \lambda V$ in (1) and (6) and expanding the λ 's in power series in λ , i.e.:

$$a_j = a_j^{(0)} + \lambda a_j^{(1)} + \lambda^2 a_j^{(2)} + \dots$$

We assume that these series are analytic for λ between 0 and 1. We can therefore substitute in (6), equate coefficients of equal powers of λ and set

$\lambda = 1$ in the final results. Then:

$$\begin{aligned} \dot{a}_k^{(0)} + \lambda \dot{a}_k^{(1)} + \lambda^2 \dot{a}_k^{(2)} + \dots &= -i \sum_j (a_j^{(0)} + \lambda a_j^{(1)} + \dots) \lambda V_{kj} e^{i\omega_{kj} t} \\ \therefore a_k^{(0)} &= \text{constant} \\ \dot{a}_k^{(s+1)} &= -i \sum_j a_j^{(s)} V_{kj} e^{i\omega_{kj} t} \quad (s = 0, 1, 2, \dots) \end{aligned} \quad (18)$$

These equations permit, in principle, obtain approximate solutions to any desired order in the perturbation.

The values of $a_k^{(0)}$ are the initial conditions of the problem: $a_k^{(0)} = c_k$ (states before the perturbation is applied). We assume all, except one of the $a_k^{(0)}$ are zero, i.e. the system is initially in a definite energy state. Then:

$$a_k^{(0)} = \delta_{km} \quad (m = \text{initial state})$$

At first order we have:

$$\dot{a}_k^{(1)} = -i V_{km} e^{i\omega_{km} t}$$

$$\therefore a_k^{(1)} = -i \int_0^t V_{km}(t') e^{i\omega_{km} t'} dt' \quad (9)$$

Note that $a_k^{(1)}$ must be zero before the perturbation is applied. If we take:

$$V = \begin{cases} 0 & \text{for } t < 0 \\ \text{constant} & \text{for } t > 0 \end{cases}$$

the integral (9) yields:

$$a_k^{(1)} = -V_{km} \frac{e^{i\omega_{km} t} - 1}{i\omega_{km}}$$

Then, the probability of finding the system, in the state k at time t is:

$$|a_k^{(1)}|^2 = 2|V_{km}|^2 \frac{1 - \cos \omega_{km} t}{\omega_{km}^2}$$

In the limit $t \rightarrow \infty$, since:

$$\lim_{t \rightarrow \infty} \frac{1 - \cos x}{x^2 t} = \pi \delta(x)$$

we obtain, for the transition probability per unit time:

$$w = \frac{1}{t} |a_k^{(1)}|^2 = 2\pi |V_{km}|^2 \delta(E_k - E_m)$$

If we take:

$$V = \begin{cases} e^{xt} C & \text{for } t < 0 \\ C & \text{for } t > 0 \end{cases}$$

with $x > 0$ and $C = \text{constant}$ we have for the integral (9):

$$a_k^{(1)} = -V_{km} \frac{e^{i\omega_{km} t}}{\omega_{km}}$$

Schrodinger Theory

Résumé of Time-independent Perturbation Theory

1. Transition Probability (Time-independent perturbation theory)
Let us consider a system whose Hamiltonian can be written as:

$$H = K + V \quad (1)$$

The eigenfunctions of this Hamiltonian satisfy the Schrödinger equation:

$$i\partial_t |\Psi\rangle = H |\Psi\rangle \quad (2)$$

For the energy E_j we can write its time-dependent solutions as:

$$|\Psi_j\rangle = e^{-iE_j t} |\Phi_j\rangle \quad (3)$$

where the time-independent part satisfies the equation:

$$H |\Phi_j\rangle = E_j |\Phi_j\rangle \quad (4)$$

Now we assume we know the solutions for the part K of the hamiltonian. These are solutions of:

$$K |\Phi_j\rangle = E_j |\Phi_j\rangle \quad (5)$$

(and we can call them unperturbed time-independent solutions) with the following properties:

$$\left. \begin{array}{l} \text{Orthonormality: } \langle \Phi_i | \Phi_j \rangle = \delta_{ij} \\ \text{Completeness: } \sum_k |\Phi_k\rangle \langle \Phi_k| = 1 \end{array} \right\} \quad (6)$$

From (4) we have:

$$(E_j - K) |\Phi_j\rangle = V |\Phi_j\rangle \quad (7)$$

and expanding in terms of Φ 's

$$|\Phi_j\rangle = \sum_k |\Phi_k\rangle \langle \Phi_k | \Phi_j \rangle$$

Substituting in (7) it yields:

$$\sum_k (E_j - E_k) |\Phi_k\rangle \langle \Phi_k | \Phi_j \rangle = V |\Phi_j\rangle$$

and using (6) we obtain:

$$(E_j - E_i) \langle \Phi_i | \Phi_j \rangle = \langle \Phi_i | V | \Phi_j \rangle \equiv T_{ij} \quad (8)$$

$$\therefore \langle \Phi_k | \Phi_j \rangle = \frac{T_{kj}}{E_j - E_k} = \frac{\langle \Phi_k | V | \Phi_j \rangle}{E_j - E_k}$$

$$\text{and then: } |\Phi_j\rangle = \sum_k \frac{|\Phi_k\rangle \langle \Phi_k | V | \Phi_j \rangle}{E_j - E_k} = G(E_j) V |\Phi_j\rangle \quad (9)$$

$$\text{where: } G(E_j) \equiv \sum_k \frac{|\Phi_k\rangle \langle \Phi_k|}{E_j - E_k} \quad (10)$$

is the Green's function.

Then, the general solution of the equation (7) is:

$$|\Psi_j\rangle = |\Phi_j\rangle + G(E_j) V |\Phi_j\rangle \quad (11)$$

(sum of a solution of the homogeneous equation plus a particular solution of the inhomogeneous). In order to define the solutions (11) we need to include the boundary conditions. We claim for outgoing waves as solutions. Then we must take the Green's function

$$G^{(+)}(E) \equiv \lim_{\epsilon \rightarrow +0} \sum_k \frac{|\Phi_k\rangle \langle \Phi_k|}{E - E_k + i\epsilon} \quad (12)$$

Then, the correct time-independent solution is:

$$|\Psi_j^{(+)}\rangle = |\Phi_j\rangle + G^{(+)}(E_j) V |\Phi_j^{(+)}\rangle \quad (13)$$

We can obtain approximated solutions by iteration of this equation:

$$|\Psi_j^{(+)}\rangle = |\Phi_j\rangle + G^{(+)}(E_j) V |\Phi_j\rangle + G^{(+)}(E_j) V G^{(+)}(E_j) V |\Phi_j\rangle + \dots$$

We remark now that the time-dependent solutions are:

$$|\Psi_j\rangle = e^{-iE_j t} |\Phi_j\rangle \quad |\Phi_j\rangle = e^{-iE_j t} |\Psi_j\rangle$$

define the S matrix as

$$\langle \Phi_i | \Phi_j \rangle = \delta_{ij} + \langle \Phi_i | G^{(+)}(E_j) V | \Phi_j \rangle e^{-i(E_j - E_i)t} = \delta_{ij} + \frac{e^{-i(E_j - E_i)t}}{E_j - E_i + i\epsilon} T_{ij}$$

But: (Cf. Jauch and Rohrlich p. 464)

$$\lim_{\epsilon \rightarrow +0} \frac{e^{-i\omega t}}{\omega + i\epsilon} = -2\pi i \delta(\omega) \quad (14)$$

Then the transition amplitude, when $t \rightarrow +0$, we can show:

$$\langle \Phi_i | \Phi_j \rangle = \delta_{ij} - 2\pi i \delta(E_i - E_j) T_{ij} \quad (15)$$

It is interesting remark the formal procedure: from equation (7) we can write:

$$|\Phi_j\rangle = |\Phi_j\rangle + \frac{1}{E_j - K} V |\Phi_j\rangle \quad (16)$$

where $G(E) \equiv \frac{1}{E - K}$

is the Green's function; from this it follows:

$$\langle \Phi_i | \Phi_j \rangle = \delta_{ij} + \langle \Phi_i | \frac{1}{E_j - K + i\epsilon} V | \Phi_j \rangle = \delta_{ij} + \frac{e^{-i(E_j - E_i)t}}{E_j - E_i + i\epsilon} T_{ij}$$

Sometimes is useful define the operator Ω (called the wave operator) as:

$$\mathcal{L}^{(+)} |\phi_i\rangle \equiv |\psi_j^{(+)}\rangle \quad (17)$$

Note that this operator satisfies (from (13)):

$$\mathcal{L}^{(+)} = 1 + G^{(+)}(E_f) V \mathcal{L}^{(+)} \quad \text{and} \quad \langle \psi_i^{(-)} | \mathcal{L}^{(+)} \rangle = \langle \psi_i^{(-)} | \mathcal{L}^{(+)} | \psi_j^{(+)} \rangle =$$

2. S-matrix formalism (Time-dependent perturbation theory) = $\langle \phi_i | S | \phi_f \rangle$
Let us consider again the equation (2). We'll change now to the interaction picture. For this we do:

$$|\Psi\rangle = e^{-i\mathcal{L}t} |\psi(t)\rangle \quad (18)$$

and substituting in (2) we obtain the equation of motion in interaction picture:

$$i\partial_t |\psi(t)\rangle = V(t) |\psi(t)\rangle \quad (19)$$

where: $V(t) \equiv e^{-i\mathcal{L}t} V e^{-i\mathcal{L}t}$ (20)

These time-dependent solutions can be written as:

$$|\psi(t)\rangle = V(t) |\phi_i\rangle \quad (21)$$

where $|\phi_i\rangle \equiv |\psi(-\infty)\rangle$. The operators V have the properties:

$$\begin{aligned} V^+ V &= V V^+ = 1 \\ V(-\infty) &= 1 \end{aligned} \quad \left. \right\} \quad (22)$$

(the first relation express the probability conservation law and the second is the boundary condition for $t=-\infty$). Furthermore, the V 's satisfy the Schrödinger equation:

$$i\partial_t V = V(t) V \quad (23)$$

The solution of this equation is obtained integrating. So

$$V(t) = 1 - i \int_{-\infty}^t V(t') V(t') dt' \quad (24)$$

We can expand this equation by induction.

We define the S-matrix as: $V(t) = 1 - i \int_{-\infty}^t V(t') dt' - \int_{-\infty}^t \int_{-\infty}^{t'} V(t') V(t'') dt' dt''$
 $S \equiv V(+\infty)$ and then obtain a expansion (25)

for the S. (Cf. Lippmann-Schwinger notes eq (25))

$$|\phi_f\rangle = |\psi(+\infty)\rangle = S |\phi_i\rangle \quad (26)$$

From (24) we have:

$$S = 1 - i \int_{-\infty}^{\infty} V(t') V(t') dt' \equiv 1 + T \quad (27)$$

In terms of the S-matrix the transition amplitude is:

$$\langle \phi_i | S | \phi_f \rangle = \delta_{if} - i \int_{-\infty}^{\infty} \langle \phi_i | V(t') V(t') | \phi_f \rangle dt'$$

But:

$$\begin{aligned} \langle \phi_i | V(t') V(t') | \phi_f \rangle &= \langle \phi_i | e^{i\mathcal{L}t'} V e^{-i\mathcal{L}t'} V(t') | \phi_f \rangle = \\ &= e^{i\mathcal{L}t'} \langle \phi_i | V | \phi_f \rangle = e^{i(E_i - E_f)t'} \langle \phi_i | V | \phi_f \rangle = \\ &= e^{i(E_i - E_f)t'} T_{if} \\ \therefore \langle \phi_i | S | \phi_f \rangle &= \delta_{if} - i T_{if} \int_{-\infty}^{\infty} e^{i(E_i - E_f)t'} dt' = \delta_{if} - 2\pi i \delta(E_i - E_f) T_{if} \end{aligned}$$

Then:

$$(S)_{if} = \delta_{if} - 2\pi i \delta(E_i - E_f) T_{if} \quad (28)$$

and:

$$(T)_{if} \equiv -2\pi i \delta(E_i - E_f) T_{if} \quad (29)$$

where $T_{if} = \langle \phi_i | V | \phi_f \rangle = \langle \phi_i | V | \phi_f \rangle + \langle \phi_i | V G^{(+)}(E_f) V | \phi_f \rangle$
 $= \langle \phi_i | V | \phi_f \rangle + \langle \phi_i | V G^{(+)}(E_f) V | \phi_f \rangle + \langle \phi_i | V G^{(+)} V G^{(+)} V | \phi_f \rangle + \dots$

In terms of diagrams this expansion is:

$$\langle i | V | f \rangle = \sum_{m,n} \langle i | V | m \rangle \langle m | G^{(+)} | n \rangle \langle n | V | f \rangle$$

In operational notation, the above results are:

$$S = 1 + T$$

$$T = -2\pi i \delta(E_i - E_f) T = -2\pi i \delta(\Delta E) T$$

and:

~~$T = T_{if} \delta(E_i - E_f)$~~

$$\text{or: } T = V + V G^{(+)} V + V G^{(+)} V G^{(+)} V + \dots$$

3. Cross Sections

From (28) we have for the transition probability:

$$W_{if} = 4\pi^2 |\delta(E_i - E_f) T_{if}|^2 \quad \text{for } i \neq f \quad (30)$$

Using the relation:

$$\delta(\omega) = (2\pi)^2 \int_{-\infty}^{\infty} e^{i\omega t} dt$$

we have:

$$|\delta(E_i - E_f)|^2 = (2\pi)^2 \delta(E_i - E_f) \int_{-\infty}^{\infty} e^{i(E_i - E_f)t} dt = (2\pi)^2 \delta(E_i - E_f) \int_{-\infty}^{\infty} dt$$

Then, the transition rate is:

$$W_{if} = 2\pi \delta(E_i - E_f) |T_{if}|^2 \quad (31)$$

Actually we have transitions to groups of states in the neighbourhood of E_f . If $\rho_{fd} dE_f$ is the number of states in dE_f , the transition rate will be:

$$W_{if} = 2\pi |T_{if}|^2 P_f$$

is $\frac{1}{(2m)^3} v^3$ (since our wave functions are $\phi_k = (2\pi)^{-\frac{3}{2}} e^{ik \cdot r}$) where v is the incident flux ~~is numerically~~ the velocity of the incident particle in the Center of Mass system. Then the cross section is:

$$\sigma_{if} = \frac{(2\pi)^3}{v} W_{if}$$

$$\therefore \sigma_{if} = \frac{(2\pi)^4}{v} |T_{if}|^2 P_f \quad (32)$$

We define the reaction operator K as the hermitian operator:

$$K = 2i \frac{S-1}{S+1} \quad (33)$$

Then: $S = \frac{1 - \frac{1}{2}iK}{1 + \frac{1}{2}iK} \quad (34)$

Since S is unitary we can introduce the hermitian operator δ as:

$$S = e^{2i\delta} \quad (35)$$

Then: $T = S-1 = 2i e^{i\delta} \sin \delta \quad (36)$

and: $K = -2 \tan \delta \quad (37)$

From: $SS^+ = 1$ we obtain:

$$(1+T)(1+T^+) = 1$$

$$\therefore T^+T = -(T+T^+) \quad (38)$$

We write this relation in terms of matrix elements: From (29):

$$4\pi^2 \sum_k \delta(E_i - E_k) T_{ik} \delta(E_j - E_k) T_{jk}^* = 2\pi i \delta(E_i - E_j) (T_{ij} - T_{ji}^*)$$

For $i=j$, i.e at forward direction:

$$2\pi \sum_k \delta(E_i - E_k) |T_{ik}|^2 = -2 \Im T_{ii}$$

and from (37) we have:

$$\sum_k W_{ik} = -2 \Im T_{ii} \quad (39)$$

relation known as the Optical Theorem.

We derive now the usual formulas for scattering. Let us take a Schrödinger representation for the integral equation for scattering (13):

$$\langle \Sigma | \psi_j \rangle = \langle \Sigma | \phi_j \rangle + \langle \Sigma | G^{(+)}(E_j) V | \psi_j \rangle = \langle \Sigma | \phi_j \rangle + \sum_k \frac{\langle \Sigma | \phi_j \rangle \langle \phi_k | V | \psi_j \rangle}{E_j - E_k + i\epsilon}$$

or, in the usual notation :

$$\psi_j(\Sigma) = \phi_j(\Sigma) + \int G_j^{(+)}(\Sigma, \Sigma') V(\Sigma') \psi_j(\Sigma') d\Sigma' \quad (40)$$

where the Green's function is:

$$G_j^{(+)}(\Sigma, \Sigma') \equiv \sum_k \frac{\phi_k(\Sigma) \phi_k^*(\Sigma')}{E_j - E_k + i\epsilon} \quad (41)$$

We can evaluate this expression as follows:

Since: $\phi_k(\Sigma) = (2\pi)^{-\frac{3}{2}} e^{ik \cdot \Sigma}$ (where $k^2 = 2mE$) we have:

$$G_j^{(+)}(\Sigma, \Sigma') = \frac{m}{8\pi^3} \int \frac{e^{ik \cdot (\Sigma - \Sigma')}}{(k_j + i\epsilon)^2 - k^2} dk = \\ = \frac{m}{4\pi^3} \int_0^\infty \int_0^{2\pi} \int_0^\pi \frac{e^{ik \cos \theta}}{(k_j + i\epsilon)^2 - k^2} k^2 dk \sin \theta d\theta d\phi$$

where $\underline{\Omega} \equiv \Sigma - \Sigma'$ and θ is the angle between \underline{k} and $\underline{\Omega}$.

Integrating we have:

$$G_j^{(+)}(\Sigma, \Sigma') = \frac{m}{\pi^2 g} \int_0^\infty \frac{K \sin K}{(k_j + i\epsilon)^2 - K^2} dK = \frac{m}{2\pi^2 g} I$$

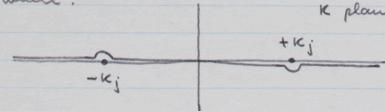
where $K \equiv k_j$ $K_j = k_j g$ and the integral.

$$I = 2 \int_0^\infty \frac{K \sin K}{(k_j + i\epsilon)^2 - K^2} dK$$

can be evaluated as the integral:

$$I = \int_C \frac{K \sin K}{k_j^2 - K^2} dK$$

where:



By the well-known method of residues we obtain:

$$I = \int_C \frac{K \sin K}{k_j^2 - K^2} dK = \frac{1}{2i} \left[\int_C \frac{K e^{ik}}{(k_j - \epsilon)(k_j + \epsilon)} dk - \int_C \frac{K e^{-ik}}{(k_j - \epsilon)(k_j + \epsilon)} dk \right] = \\ = -\pi e^{ik_j} = I$$

Then, finally:

$$G_j^{(+)}(\Sigma, \Sigma') = -\frac{m}{2\pi} \frac{e^{ik_j |\Sigma - \Sigma'|}}{|\Sigma - \Sigma'|} \quad (42)$$

From (40), cancelling out the indices, we have:

$$\psi(\underline{r}) = \phi(\underline{r}) - \frac{m}{2\pi} \int \frac{e^{ik|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|} V(\underline{r}') \psi(\underline{r}') d\underline{r}' \quad (43)$$

This is nothing else than the integral equation corresponding to Schrödinger equation as we can easily see. Rewriting the time-independent Schrödinger equation as an inhomogeneous Helmholtz equation we have:

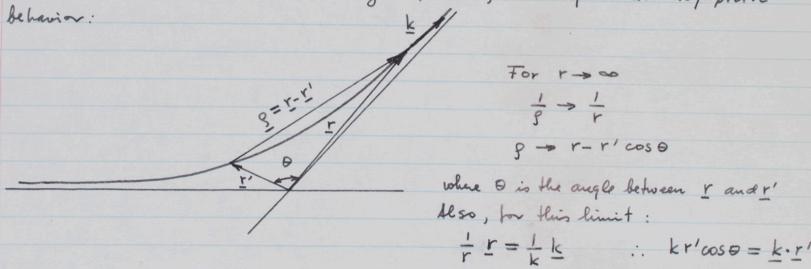
$$\Delta \psi + k^2 \psi = 2mV(\underline{r}) \psi$$

and its solution is the sum of a solution of the homogeneous equation (i.e. a free particle solution ϕ) plus a solution of the inhomogeneous equation, which can be constructed using the Green's function for the Helmholtz equation satisfying the required boundary conditions, i.e.:

$$G(\underline{r}, \underline{r}') = \frac{1}{4\pi} \frac{e^{ik|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|} \quad (44)$$

Clearly, this solution is (43).

In order to obtain the scattering amplitude, we study now its asymptotic behavior:



Then, the equation (43) tends to:

$$\begin{aligned} \psi(\underline{r}) &\rightarrow \phi(\underline{r}) - \frac{m}{2\pi} \frac{e^{ikr}}{r} \int e^{-ik|\underline{r}'|} V(\underline{r}') \psi(\underline{r}') d\underline{r}' = \\ &= (2\pi)^{-\frac{3}{2}} \left[e^{ik \cdot \underline{r}} - 4\pi^2 m \frac{e^{ikr}}{r} \int \phi(\underline{r}') V(\underline{r}') + (\underline{r}') d\underline{r}' \right] \end{aligned}$$

$$\therefore \psi(\underline{r}) \xrightarrow[r \rightarrow \infty]{} (2\pi)^{-\frac{3}{2}} \left[e^{ik \cdot \underline{r}} - 4\pi^2 m \langle \phi | V | \psi \rangle + \frac{e^{ikr}}{r} \right] \quad (45)$$

Therefore, the scattering amplitude is: (Cf. Schiff p. 102):

$$f(\theta, \phi) = -4\pi^2 m \langle \phi | V | \psi \rangle = -\sqrt{2\pi} m \int e^{-ik|\underline{r}'|} V(\underline{r}') + (\underline{r}') d\underline{r}' \quad (46)$$

Clearly here, θ and ϕ are the angles of direction of vector \underline{k} , i.e. the scattering direction (in C. of mass system, of course). Note also that the coefficient of matrix element depends on the normalization chosen for the wave functions. We are using the S normalization. We could obtain this result using the general

formalism as we will see now. The density ρ_f of final states into the solid angle $d\Omega$ around the direction θ, ϕ is:

$$dp dE = \frac{V p^2 d\rho d\Omega}{8\pi^3} \quad (47)$$

where V is the spatial volume. This volume is $V = (2\pi)^3$ since the wave functions are normalized in the S normalization. ($\phi = (2\pi)^{-\frac{3}{2}} e^{ik \cdot \underline{r}}$ gives a fraction $(2\pi)^{-3}$ of particle per unit volume. Note that if we were used the box normalization: $\phi = L^{-\frac{3}{2}} e^{ik \cdot \underline{r}}$, the volume would be L^3 , the volume of the box). Since

$$E = \frac{p^2}{2m} \quad dE = \frac{p}{m} dp.$$

Then: $d\rho = mp d\Omega = m^2 v d\Omega$ (48)
From (32), we have for the differential cross-section:

$$d\sigma = \frac{(2\pi)^4}{V} |T_{if}|^2 d\Omega$$

$$\therefore \frac{d\sigma}{d\Omega} \equiv |f(\theta, \phi)|^2 = m^2 (2\pi)^4 |T_{if}|^2$$

and $f = -4\pi^2 m T_{if}$, eq. (46) (the sign - is by definition). If we put $\psi \approx \phi = (2\pi)^{-\frac{3}{2}} e^{ik \cdot \underline{r}}$ in the scattering amplitude, we obtain:

$$f(\theta, \phi) = -\frac{m}{2\pi} \int e^{i(k_f - k_i) \cdot \underline{r}'} V(\underline{r}') d\underline{r}' \quad (49)$$

the Born approximation. (Cf. Morse and Feshbach p. 1069 and Schiff p. 159). In terms of the scattering amplitude the optical theorem is:

$$\sum_f \sigma_f \equiv \sigma_{tot} = -2 \frac{(2\pi)^3}{V} \Im T_{ii} = -2 \frac{(2\pi)^3}{V} \left(-\frac{1}{4\pi^2 m} \right) \Im f(0)$$

$$\therefore \sigma_{tot} = \frac{4\pi}{k} \Im f(0) \quad (50)$$

Scattering of a particle by a fixed potential.

$$\text{Hamiltonian: } H = H_0 + V \quad V = V(r) \quad (1)$$

$$H_0 = \frac{k^2}{2m} \cdot \cancel{\int d\vec{r} \frac{V(\vec{r})}{8\pi^3} e^{-ik\cdot\vec{r}}} \rightarrow$$

Unperturbed states:

$$|k\rangle \equiv \frac{1}{\sqrt{8\pi^3}} e^{ik\cdot\vec{r}} \quad (2)$$

$$H_0|k\rangle = E_k|k\rangle$$

$$\langle k'|k\rangle = \delta(k' - k) \quad (3)$$

Resident:

$$R(z) \equiv (H-z)^{-1} \quad z = \text{complex.} \quad (4)$$

$$H_0 - z = H - z - V$$

$$\therefore R(z) = \frac{1}{H_0 - z} (H - z - V)$$

$$\text{or: } R(z) = \frac{1}{H_0 - z} (H - z - V) R(z) = \frac{1}{H_0 - z} - \frac{1}{H_0 - z} V R(z)$$

$$\therefore R(z) = \frac{1}{H_0 - z} - \frac{1}{H_0 - z} V R(z) \quad (5)$$

Iterating:

$$R(z) = \frac{1}{H_0 - z} - \frac{1}{H_0 - z} V \frac{1}{H_0 - z} + \frac{1}{H_0 - z} V \frac{1}{H_0 - z} V \frac{1}{H_0 - z} - \dots \quad (6)$$

Calculating:

$$\langle k'|R(z)|k\rangle = \frac{1}{E_k - z} \delta(k' - k) - \frac{1}{E_{k'} - z} \langle k'|K(z)|k\rangle \frac{1}{E_k - z} \quad (6')$$

where:

$$\langle k'|K(z)|k\rangle = \langle k'|[V - V \frac{1}{H_0 - z} V + \dots] |k\rangle \quad (7)$$

Note $\langle k'|R(z)|k\rangle$ and $\langle k'|K(z)|k\rangle$ have singularities only on the real axis.

From (7):

$$\langle k'|K(z)|k\rangle = \langle k'|V|k\rangle - \int dk_1 \frac{\langle k'|V|k_1\rangle \langle k_1|V|k\rangle}{E_{k_1} - z} + \dots \quad (8)$$

$$\text{But: } \langle k'|V|k\rangle = \frac{1}{8\pi^3} \int d\vec{r} e^{i(k-k')\cdot\vec{r}} V(r) = V(k-k') \quad (9)$$

The 2nd term of (8) becomes:

$$\int dk_1 \frac{V(k'-k_1) V(k_1 - k)}{k_1^2/2m - z} \rightarrow \int dk \frac{k^2 f(k)}{k^2 - z}$$

This int. has two limits: $z = a + i\epsilon$ ($a > 0$)

From (6') these limits yields:

$$\lim_{z \rightarrow E_k \pm i0} \langle k'|R(z)|k\rangle (E_k - z) \equiv \langle k'|U_k^\pm|k\rangle$$

$$\therefore U_k^\pm = \lim_{z \rightarrow E_k \pm i0} (E_k - z) R(z) |k\rangle \quad (10)$$

$$H - E_k - (H - z) = z - E_k$$

$$\therefore (H - E_k)(E_k - z) R(z) |k\rangle - (E_k - z) |k\rangle = -(E_k - z)^2 R(z) |k\rangle$$

$$\text{Taking } \lim_{z \rightarrow E_k \pm i0} : (H - E_k) |U_k^\pm|k\rangle = 0 \quad (11)$$

From (6) and (10):

$$\langle k'|U_k^\pm|k\rangle = \delta(k' - k) + \frac{1}{E_k^\pm - E_k} \langle k'|U_k^\pm|k\rangle \quad (12)$$

The matrices: U_k^\pm

$$\langle k'|K^\pm|k\rangle \equiv \lim_{z \rightarrow E_k \pm i0} \langle k'|K(z)|k\rangle$$

are called scattering matrices and satisfy the eq:

$$\langle k'|K^\pm|k\rangle = \langle k'|V|k\rangle + \int dk'' \frac{\langle k'|V|k''\rangle \langle k''|K^\pm|k\rangle}{E_k^\pm - E_{k''}} \quad (13)$$

The time-dependent wave function is:

$$|U_k^\pm(t)\rangle = e^{-iE_k t} |U_k^\pm\rangle$$

$$|\psi_k^+(t)\rangle = e^{-iE_k t} |\psi_k^+\rangle$$

and a wave packet:

$$\begin{aligned} |\psi^+(t)\rangle &= \int dk' C_{k'} |\psi_{k'}^+(t)\rangle = \int dk' C_{k'} e^{-iE_{k'} t} |\psi_{k'}^+\rangle = \\ &= \int dk' |k'\rangle e^{-iE_{k'} t} \int dk'' C_{k''} e^{-i(E_k - E_{k'}) t} \langle k''| \psi_{k'}^+ \rangle = \\ &= \int dk' Y_{k'}(t) e^{-iE_{k'} t} |k'\rangle \end{aligned}$$

where:

$$Y_{k'}(t) = \int dk'' C_{k''} e^{-i(E_k - E_{k''}) t} \langle k''| \psi_{k'}^+ \rangle$$

From (12):

$$Y_{k'}(t) = \int dk'' C_{k''} [\delta(k - k'') + \frac{e^{-i(E_k - E_{k''}) t}}{E_{k''} - E_k} \langle k''| K^+ |k\rangle]$$

But:

$$\lim_{t \rightarrow -\infty} \frac{e^{-iE_k t}}{E_k} = 0$$

$$\therefore \lim_{t \rightarrow -\infty} Y_{k'}(t) = C_k$$

$$\therefore |\psi^+(t)\rangle \equiv \int dk' C_{k'} e^{-iE_{k'} t} |\psi_{k'}^+\rangle \xrightarrow[t \rightarrow -\infty]{} |\phi(t)\rangle \equiv \int dk' C_{k'} e^{-iE_{k'} t} |\psi_{k'}^+\rangle$$

$|\psi_k^+\rangle$ describes a state where the incoming particle is in a plane wave state. Symbolically: $|\psi_k^+\rangle \xrightarrow[t \rightarrow -\infty]{} |k\rangle$

Now:

$$\lim_{t \rightarrow +\infty} \frac{e^{-iE_k t}}{E_k} = -2\pi i \delta(E)$$

$$\therefore \lim_{t \rightarrow +\infty} Y_{k'}(t) = \int dk'' C_{k''} [\delta(k - k'') - 2\pi i \delta(E_k - E_{k''}) \langle k''| K^+ |k\rangle]$$

$$\text{But: } |\psi_k^+\rangle \xrightarrow[t \rightarrow +\infty]{} S_{kk'} |k'\rangle$$

where $S_{kk'}$ is the S-matrix. Hence:

$$S_{kk'} = S(k - k') - 2\pi i \delta(E_k - E_{k'}) \langle k'| K^+ |k\rangle$$

Now:

$$\langle k'| V | \psi_k^+ \rangle = \int dk'' \langle k'| V | k'' \rangle \langle k''| \psi_k^+ \rangle$$

From (12) and (13):

$$\langle k'| V | \psi_k^+ \rangle = \langle k'| K^+ |k\rangle$$

$$\text{or: } (E_k - E_{k'}) \langle k'| \psi_k^+ \rangle = \langle k'| K^+ |k\rangle$$

From (10) and (6) we get:

$$\langle k'| K^+ |k\rangle = \langle k'| V |k\rangle + \langle k'| V \frac{1}{E_k^+ H_0} V |k\rangle + \dots$$

Scattering by two potentials.

$$\Psi^+ = \Phi + \frac{1}{\epsilon_i^+ - \tau} (U + V) \Psi_i^+$$

$$\Lambda^\pm = \Phi + \frac{1}{\epsilon_i^\pm - \tau} U \Lambda_i^\pm$$

1) Lemma:

$$\langle \Lambda_f^-, U \Phi_i \rangle = \langle \Phi_f, U \Lambda_i^+ \rangle \quad \text{on the energy shell. } (\epsilon_i = \epsilon_f)$$

Proof:

$$\begin{aligned} \langle \Lambda_f^-, U \Phi_i \rangle &= \langle \Lambda_f^-, U \left(1 - \frac{1}{\epsilon_i^+ - \tau} U\right) \Lambda_i^+ \rangle = \langle \Lambda_f^-, U \Lambda_i^+ \rangle - \langle \frac{1}{\epsilon_i^+ - \tau} U \Lambda_f^-, U \Lambda_i^+ \rangle \\ &= \langle \Lambda_f^-, U \Lambda_i^+ \rangle - \langle (\Lambda_f^- - \Phi_f), U \Lambda_i^+ \rangle = \langle \Phi_f, U \Lambda_i^+ \rangle \quad \blacksquare \end{aligned}$$

2) Theorem:

$$\langle \Phi_f, (U + V) \Psi_i^+ \rangle = \langle \Phi_f, U \Lambda_i^+ \rangle + \langle \Lambda_f^-, V \Psi_i^+ \rangle \quad \text{on the energy shell.}$$

Proof:

$$\begin{aligned} \langle \Phi_f, (U + V) \Psi_i^+ \rangle &= \left\langle \left(1 - \frac{1}{\epsilon_i^+ - \tau} U\right) \Lambda_f^-, (U + V) \Psi_i^+ \right\rangle = \\ &= \langle \Lambda_f^-, \left[U + V - U \frac{1}{\epsilon_i^+ - \tau} (U + V) \right] \Psi_i^+ \rangle = \\ &= \langle \Lambda_f^-, (U + V) \Psi_i^+ \rangle - \langle \Lambda_f^-, U (\Psi_i^+ - \Phi_i) \rangle = \\ &= \langle \Lambda_f^-, V \Psi_i^+ \rangle + \langle \Lambda_f^-, U \Phi_i \rangle = \\ &= \langle \Lambda_f^-, V \Psi_i^+ \rangle + \langle \Phi_f, U \Lambda_i^+ \rangle \quad \blacksquare. \end{aligned}$$