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THE OPERATOR FORMALISM IN QUANTUM PERTURBATION THEORY

Bryce S. DeWitt

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Table of Contents

Introduction 1

1. Fundamentals 5

The perturbation operator. 5

The dynamical equations. 5

Basic commutation relations. 6

The Heisenberg representation. 6

The Schrödinger representation. 7

The interaction representation. 10

Iteration formulae. 11

H_0 independent of t. 12

Transition probabilities. 14

2. Green's functions and Fourier transforms. 16

Temporal switching operators. 16

Switching operators are Green's functions. 16

Fourier transforms. 17

Algebraic relations. 18

Time independence. 19

3. Types of systems. 20

Classification of states. 20

Simple and complex systems. 20

Separable Hamiltonians. 21

A special example. 22

The basic spectral types. 26

4. Simple scattering. 30

Confined forces. 30

Retarded waves. 30

Wave packets. 31

Definition of $|\text{ret}'\rangle$. 33

Advanced waves. 34

The scattering operator. 35

5. Limiting procedures. 38

Adiabatic switching. 38

Convergence of the series (5.5). 41

Passage to the limit $\epsilon \to 0$. 42

Analytic continuation. 43

Alternative limiting procedure. 44

Conventions to be adopted. 45

6. Level shifts. 47

Construction of the eigenvectors of H. 47

The normalization constant. 49

The case of bound states. 49

Remaining arbitrariness. 51

Oscillating factors. 53

Rigorous derivation of Eq. (6.24). 55

Some remarks. 57

7. Scattering continued. 59

The orthonormality of the vectors $|J_\pm'\rangle$. 59

Proof of Eq. (7.13) in the case of simple scattering. 61

The case $Z' < 1$. 63

Orthogonality of $|S_\pm'$ and $|J'\rangle$. 65

Questions of unitarity. 66

Structure of the S-matrix. 68

The reactance operator. 71

The phase shift operator. 72

Integral forms. 73

Recurrence formulae for $\underset{\sim}{K}$ and S. 75

Alternative definition of $\underset{\sim}{K}$. 77

8. Cross sections. 81

Return to the wave packet picture. 81

Transition rates and the angular cross section. 85

Derivation based on the S-matrix. 88

The connection between transition rates and the S-matrix. 90

The total cross section. 93

The case N = 1. Transmission and reflection coefficients. 94

Phase shift formulae. 95

The case of spherical symmetry. 97

Phase shifts in one dimension. 97

Two dimensions. 100

Three dimensions. 100

The reverse scattering theorem. 102

The one-dimensional delta-function potential. 103

9. Bound state perturbation theory. 107

The use of contour integration. 107

Series expansions. 109

Computation of $|J'\rangle$ and $\Delta E'$. 111

Progressive removal of degeneracy. 113

The Rayleigh-Schrödinger perturbation formula. 115

Connection with the adiabatic switching formalism 116

Convergence of the series expansions. 119

Alternative formulations. 121

The Fredholm method. 125

The adiabatic theorem. 127

The creation of bound states from free states. 129a

10. Simple field theories. 135

The nonrelativistic extended source model. 135

A condensed notation. 137

The particle propagation functions. 141

Diagrams. 144

A variational technique 148

Symmetric theories. 153

The structure of the modified nucleon propagation function. 155

Renormalization. 157

The S-matrix. 162

The reactance operator. 169

Experimental determination of the renormalized coupling constant. 173

Fourier transforms. 181

Some remarks. 184

The neutral scalar field. 185

11. Decaying systems and resonance scattering. 194

Unstable states. 194

The damping operator. 195

Real solutions. 197

Complex solutions. 198

Discussion of instability. 204

The decay process. 207

Natural line breadth. 214

The S-matrix. 226

Resonance scattering. 229

The excitation process. 232

12. Problems involving several perturbations. 235

Introduction. 235

The combination of perturbations. 237

Scattering by two potentials. 240

The example of section 3. 242

Disintegrative scattering. 243

Rearrangement collisions. 246

Channels. 250

Resonances. 253

Multiple scattering. 256

Some comments. 258

13. Final remarks. 261

Acknowledgements. 268

Bibliography. 269

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Bryce S. DeWitt

Radiation Laboratory, Department of Physics
University of California, Berkeley, California

and

Institute for Advanced Study, Princeton, New Jersey

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ABSTRACT

This article is a review of formal perturbation theory as it has been developed in the past few years. Most of the important formulae found in the literature are presented. The emphasis is on showing that the formal theory provides an adequate skeleton on which to hang the whole of quantum perturbation theory and therefore plays a valuable unifying role. Topics to which attention is devoted include: Green's functions; scattering theory, level shifts, state vector normalization, bound state perturbation theory, renormalization theory of quantized fields, decay and resonance phenomena, and the theory of nuclear reactions.

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Bryce S. DeWitt

Radiation Laboratory, Department of Physics
University of California, Berkeley, California

and

Institute for Advanced Study, Princeton, New Jersey

INTRODUCTION

In the early days of quantum mechanics approximation methods were very largely unsystematized. Although the general classical theory of perturbations which had been developed in the 19th century for application to celestial mechanical problems could, when expressed in the language of angle and action variables, be more or less directly translated by a recipe known as the Correspondence Principle into a scheme applicable to the quantum mechanics of bound systems, the techniques introduced into the study of other systems (e.g. colliding particles; periodic structures; decaying atoms and nuclei) were much more specific to the individual problems at hand. This situation began to change as the quantum mechanical systems receiving major attention became more complex, and particularly as interest arose in the "higher approximations" of quantum field theories. In recent years increased effort has been made to generalize the earlier techniques by abstracting out of them certain common essentials. This has led gradually to a compact symbolic language which is characterized by full and uninhibited use of the abstract operator formalism. The statements in this language constitute what may be referred to as a formal perturbation theory.

Aside from a desire to introduce the symbolic language in order to express key notions in a very concise form, there has also been a hope that

the flexibility of such a language, exemplified in various formal tricks of manipulation of operators, would produce some new approximation methods or justify previously suggested ones. In fact, the search for tricks has often motivated formal developments, and these developments have consequently been somewhat erratic and scattered in the literature.

This article is an attempt to collect together the most important formulae of the operator formalism. Since, however, the results of the formal theory have generally had little more than a (perhaps disappointing) preliminary usefulness as far as practical problem solving is concerned, the emphasis here will not be on tricks but rather on showing that the formal theory provides an adequate skeleton on which to hang the whole of quantum perturbation theory and therefore plays a valuable unifying role.

In the interest of keeping the operator language flexible, rigor will be maintained only in a very loose fashion. In spite of the fact that the formalism is known to contain a number of logical traps these traps are identifiable, and one may still use the formalism in a well-defined and unambiguous way to set up the correct mathematical statement of a given specific physical problem. The mathematical operations in the specific case can then be tested for rigor. This point of view has long been well accepted (see, for example, Dirac, reference [4]).*

No attempt will be made to discuss the rather specialized covariant formal language developed by many authors [123 to 125] for use in relativistic field theories. The equations written here will remain nonrelativistic in form, although in many cases their generalization to a covariant form is perfectly

---

* References are to the bibliography at the end of the article.

straightforward. This restriction is not really serious, since many of the special features peculiar to field theories can be well illumined by the nonrelativistic formalism alone (see section 10).

In the following section the mathematical fundamentals of the operator formalism are assembled. In section 2 the basic Green's functions and their Fourier transforms are introduced. Section 3 contains a brief classification of systems according to their bound and free states and the grouping of their energy levels. The simple theory of scattering is described in section 4 and forms the point of departure for subsequent developments.

The intuitive constructs introduced in section 4 are refined in section 5 through the introduction of suitable limiting procedures. Questions of convergence are immediately encountered and are analyzed in an elementary fashion. One is led naturally to a study of level shifts, which is carried out in section 6, the important phenomenon of state-vector renormalization being simultaneously emphasized. The utility of the adiabatic switching device is also fully illustrated.

Section 7 contains simple derivations of many of the important formulae of the mathematical theory of scattering. In section 8 the method of applying these formulae to the computation of cross sections is indicated.

Section 9 consists of a fairly detailed exposition of how bound state perturbation theory fits into the general operator formalism, and how the discreteness of the energy levels modifies many of the theoretical as well as computational techniques used.

The "facts of life" of simple quantum field theories are told (in a necessarily compressed form) in section 10. The phenomena of mass and

charge renormalization and their intimate relation with state-vector renormalization is shown, the demonstrations being among the most beautiful illustrations of the power of the operator formalism.

In section 11 is presented the theory of decaying systems: line breadth, Lamb shift, resonance scattering.

In section 12, the theory of scattering by more than one potential is outlined, and the connection of this theory to the theory of nuclear reactions is briefly indicated.

Section 13 consists of a number of closing remarks, chiefly about those topics of current interest which have been necessarily omitted from the present survey.

1. FUNDAMENTALS

The perturbation operator

The motif of perturbation theory is the comparison of two physical systems, one of which is simple and the other complicated. Denote by $\underset{\sim}{H}_0$ the Hamiltonian operator of the simple system, and by $\underset{\sim}{H}$ that of the complicated one. The central role of the theory is played by the difference of these two operators,

$$\underset{\sim}{H}_1 = \underset{\sim}{H} - \underset{\sim}{H}_0 \quad , \tag{1.1}$$

which may be called the perturbation operator. In practical applications the system of interest is naturally the complicated one, and the simple system is chosen (if there is any choice) to be as similar to it as possible so that $\underset{\sim}{H}_1$ may be regarded as "small." As far as the purely formal theory is concerned, however, this is an unnecessary restriction. Any $\underset{\sim}{H}_0$ has a certain utility, if no other than that of providing a matrix representation as a basis for discussion.*

The dynamical equations

If $\underset{\sim}{F}$ is the operator corresponding to any physical "observable" of the system $\underset{\sim}{H}$, its rate of change with time (we choose units $\hbar = c = 1$) is given by

$$\dot{\underset{\sim}{F}} = -i\left[\underset{\sim}{F}, \underset{\sim}{H}\right] + \partial \underset{\sim}{F}/\partial t \quad , \tag{1.2}$$

where the partial derivative is taken with respect to any explicit dependence

---

* Both $\underset{\sim}{H}_0$ and $\underset{\sim}{H}$ must, however, operate in the same vector space. In field theories questions have been raised in connection with this point. (See references [113] and [114].)

on the time which $\underset{\sim}{F}$ may have. An immediate consequence is that $\underset{\sim}{H}$ is constant if it has no explicit dependence on t. For the present, however, we shall not make such a restriction.

Basic commutation relations

If the system $\underset{\sim}{H}$ possesses a classical analog than its operators can be constructed explicitly through use of the commutation relations

$$\left[\underset{\sim}{q}^i, \underset{\sim}{q}^j\right] = 0, \qquad \left[\underset{\sim}{q}^i, \underset{\sim}{p}_j\right] = i\,\delta^i_j, \qquad \left[\underset{\sim}{p}_i, \underset{\sim}{p}_j\right] = 0, \tag{1.3}$$

where the $\underset{\sim}{q}$'s and $\underset{\sim}{p}$'s are operators corresponding respectively to the classical coordinates and their canonically conjugated momenta. If the system possesses nonclassical elements (spin in its various forms; subsystems obeying the exclusion principle) then other well known methods of construction must be employed, but Eq. (1.2) is assumed to hold in any case. It is also to be assumed that $\underset{\sim}{H}$, $\underset{\sim}{H}_0$, $\underset{\sim}{H}_1$ are Hermitian operators.

The Heisenberg representation.

If $|\underset{\sim}{\psi}\rangle$ is the vector which describes the state of the system $\underset{\sim}{H}$, and if $\langle\underset{\sim}{\psi}|$ denotes the adjoint of this vector, then the average result of an experiment designed to measure the value of the observable $\underset{\sim}{F}$ at time t will be

$$\langle F\rangle_t = \langle\underset{\sim}{\psi}\,|\,\underset{\sim}{F}(t)\,|\,\underset{\sim}{\psi}\rangle. \tag{1.4}$$

Eqs. (1.2) and (1.4) are the fundamental equations of the Heisenberg form of quantum mechanics. The chief characteristics of this so-called Heisenberg representation are 1) the constancy of the state vectors $|\underset{\sim}{\psi}\rangle$ and 2) the change of the operators $\underset{\sim}{F}$ with time. Its utility is mainly theoretical in that it provides the closest quantum analog to the classical theory.

The Schrödinger representation.

Since an operator is a more complicated object than a vector, it is desirable to place more emphasis on the state vectors. This is accomplished by introducing the Schrödinger representation:

Define an operator function $V(t'', t')$ as the solution of the following integral equation:

$$V(t'', t') = 1 + i\int_{t'}^{t''} \underset{\sim}{H}(t)\, V(t, t')dt \,. \tag{1.5}$$

An equivalent definition is evidently

$$-i \frac{\partial}{\partial t''} V(t'', t') = \underset{\sim}{H}(t'')\, V(t'', t') \tag{1.6}$$

combined with the boundary condition

$$V(t', t') = 1 \quad \text{for all } t'. \tag{1.7}$$

Eq. (1.6) may also be written

$$i \frac{\partial}{\partial t''} V(t'', t')^* = V(t'', t')^* \underset{\sim}{H}(t'') \,, \tag{1.8}$$

where the asterisk is used to denote the Hermitian adjoint (or, in the case of numbers, the ordinary complex conjugate). Eqs. (1.6) and (1.8) together give

$$\frac{\partial}{\partial t'''} \left[V(t''', t'')^* V(t''', t') \right] = 0 \,, \tag{1.9}$$

which implies, with the aid of Eq. (1.7),

$$V(t''', t'')^* V(t''', t') = V(t'', t'')^* V(t'', t') = V(t'', t') \qquad (1.10a)$$

$$= V(t', t'')^* V(t', t') = V(t', t'')^*, \qquad (1.10b)$$

which in turn yields

$$V(t'', t''') V(t''', t') = V(t'', t') \qquad \text{for all } t''', \qquad (1.11)$$

$$V(t'', t')^* V(t'', t') = V(t'', t') V(t'', t')^* = 1 . \qquad (1.12)$$

Eq. (1.12) expresses the unitarity of $V(t'', t')$. It is important to remember that both parts of this double equation are essential to the establishment of this fact. Eq. (1.10) allows the Hermitian adjoints of Eqs. (1.5) and (1.6) to be written in the respective forms

$$V(t'', t') = 1 - i\int_{t''}^{t'} V(t'', t) \underset{\sim}{H}(t)dt , \qquad (1.13)$$

$$i \frac{\partial}{\partial t'} V(t'', t') = V(t'', t') \underset{\sim}{H}(t') . \qquad (1.14)$$

The analysis thus far has been completely general. Any operator satisfying an integral equation of the form (1.5) with an Hermitian kernel will satisfy also equations identical in form with Eqs. (1.6 - 14).

Now introduce the Schrödinger operators and state vectors by the definitions

$$F(t) \equiv V(0, t) \underset{\sim}{F}(t) V(t, 0), \qquad (1.15)$$

$$|\psi(t)\rangle \equiv V(0, t)|\underset{\sim}{\psi}\rangle . \qquad (1.16)$$

These new structures satisfy the equations

$$\dot{F} = \partial F/\partial t \,, \tag{1.17}$$

$$i \frac{d}{dt} \left|\psi(t)\right\rangle = H(t) \left|\psi(t)\right\rangle \,, \tag{1.18}$$

$$\left\langle F\right\rangle_t = \left\langle \psi(t) \middle| F(t) \middle| \psi(t)\right\rangle \,. \tag{1.19}$$

Eqs. (1.18) and (1.19) are the fundamental equations of the Schrödinger representation. Eq. (1.17) expresses the chief utility of this representation. If an operator has no explicit dependence on t then its Schrödinger form is constant in time. In particular, for a system with a classical analog the q's and p's are constant operators, and consequently coordinate and momentum representations have great and meaningful applicability in this form of quantum mechanics. Moreover, the burden of describing the dynamical behavior of a system is thrown completely onto the state vectors.

The Schrödinger state vectors at two different times are connected by a unitary transformation

$$\left|\psi(t'')\right\rangle = U(t'', t') \left|\psi(t')\right\rangle \,, \tag{1.20}$$

where the operator $U(t'', t')$ satisfies the integral equation

$$U(t'', t') = 1 - i\int_{t'}^{t''} H(t)\, U(t, t')dt \tag{1.21}$$

and its corollaries. Evidently

$$U(t'', t') = V(0, t'')\, V(t', 0) \,. \tag{1.22}$$

In general $U(t'', t')$ will not be equal to $V(t', t'')$ unless H happens to be constant in time, in which case $\left[V(0, t''), V(t', 0)\right] = 0$.

The interaction representation.

We now bring the operator $\underset{\sim}{H}_0$, or rather its Schrödinger form H_0, into the picture. The "reference system" described by H_0 is assumed to be completely solved. That is to say, the behavior of all its state vectors in the Schrödinger representation, or conversely, the behavior of all its operators in its Heisenberg representation, is known. Since one is primarily interested in the deviation in the behavior of the Schrödinger state vector of system H from that of system H_0, it is often convenient to remove from $|\psi(t)\rangle$ that part of its behavior which derives from the known properties of H_0. This can be accomplished by making a partial transformation back to the Heisenberg representation:

$$\bar{F}(t) \equiv U_0(0, t)\, F(t)\, U_0(t, 0) , \tag{1.23}$$

$$|\bar{\psi}(t)\rangle \equiv U_0(0, t)\, |\psi(t)\rangle , \tag{1.24}$$

where the operator $U_0(t'', t')$ satisfies the equation

$$U_0(t'', t') = 1 - i\int_{t'}^{t''} H_0(t)\, U_0(t, t')dt, \text{ etc.} \tag{1.25}$$

Eqs. (1.23) and (1.24) introduce what has come to be known as the interaction representation. The interaction operators and state vectors satisfy the equations

$$d\bar{F}/dt = -i\left[\bar{F}, \bar{H}_0\right] + \partial\bar{F}/\partial t , \tag{1.26}$$

$$i\frac{d}{dt}|\bar{\psi}(t)\rangle = \bar{H}_1(t)\,|\bar{\psi}(t)\rangle, \tag{1.27}$$

$$\langle F\rangle_t = \langle\bar{\psi}(t)|\,\bar{F}(t)\,|\bar{\psi}(t)\rangle . \tag{1.28}$$

The transformation from one interaction state vector to another is effected by the operator

$$\bar{U}(t'', t') \equiv U_0(0, t'')\, U(t'', t')\, U_0(t', 0) \,, \tag{1.29}$$

which satisfies the equations

$$\bar{U}(t'', t') = 1 - i\int_{t'}^{t''} \bar{H}_1(t)\, \bar{U}(t, t')dt \tag{1.30a}$$

$$= 1 + i\int_{t''}^{t'} \bar{U}(t'', t)\, \bar{H}_1(t)dt \,, \text{ etc.} \tag{1.30b}$$

If H_0 and H have no explicit time dependence then the operators $U_0(t'', t')$ and $U(t'', t')$ depend only on the difference between the times t'' and t'. It is to be noted that the operator $\bar{U}(t'', t')$, on the other hand, is never a function simply of $t'' - t'$, except in trivial cases (e.g. when H commutes with H_0).

<u>Iteration formulae.</u>

By iteration of Eqs. (1.30) one obtains, for $t'' > t'$, [11],

$$\bar{U}(t'', t') = 1 + \sum_{n=1}^{\infty} (-i)^n \int_{-\infty}^{\infty} dt_1 \ldots \int_{-\infty}^{\infty} dt_n\, \theta_+(t'' - t_1)\, \theta_+(t_1 - t_2) \ldots$$

$$\ldots \theta_+(t_{n-1} - t_n)\, \theta_+(t_n - t')\, \bar{H}_1(t_1) \ldots \bar{H}_1(t_n) \tag{1.31a}$$

$$= \left[\exp\left(-i\int_{t'}^{t''} \bar{H}_1(t)dt\right)\right]_+ \,, \tag{1.31b}$$

and, for $t'' < t'$,

$$\bar{U}(t'', t') = 1 + \sum_{n=1}^{\infty} (i)^n \int_{-\infty}^{\infty} dt_1 \ldots \int_{-\infty}^{\infty} dt_n \, \theta_-(t'' - t_1)\, \theta_-(t_1 - t_2) \ldots$$

$$\ldots \theta_-(t_{n-1} - t_n)\, \theta_-(t_n - t')\, \bar{H}_1(t_1) \ldots \bar{H}_1(t_n) \tag{1.32a}$$

$$= \left[\exp\left(i \int_{t''}^{t'} \bar{H}_1(t)dt\right)\right]_- \tag{1.32b}$$

where

$$\theta_\pm(t) \equiv \tfrac{1}{2}(1 \pm t/|t|), \tag{1.33}$$

and where the "time ordering" brackets $[\quad]_+$ and $[\quad]_-$ arrange the time dependent operators contained within them from right to left in order of increasing and decreasing values of their arguments t respectively. The second forms of Eqs. (1.31) and (1.32) are obtained from the first forms through the observation that one can permit the inclusion of all $n!$ ways of permuting the factors $\bar{H}_1(t_1) \ldots \bar{H}_1(t_n)$ (which is equivalent to omitting the functions $\theta_\pm$ and replacing the limits of integration by t' and t'') if one simply uses the time ordering brackets as a formal device to unscramble them again, and then multiplies by $1/n!$.

<u>H_o independent of t.</u>

The interaction representation is particularly useful when H_o is independent of t, as is almost always the case. The system H_o then has N independent commuting constants of motion $\alpha_o^{\,i}$ $(i = 1 \ldots N)$ where N is the number of degrees of freedom. (N may be nondenumberably infinite!)

If the system has a classical analog these constants correspond to certain independent functions of the q's and p's which have vanishing Poisson brackets with one another. For convenience the α_o^i will be denoted collectively by α_o.

The α_o are a complete set of commuting operators, and define a most useful basis in the vector space of the system H_o. Following Dirac [4] we shall use dashes to identify the eigenvalues of the α_o, the corresponding eigenvectors being denoted by $|\alpha_o'\rangle$:

$$\alpha_o |\alpha_o'\rangle = \alpha_o' |\alpha_o'\rangle \quad . \tag{1.34}$$

The α_o' may come partly from a continuum and partly from a discrete set, or all from one or the other. The most important of the different possibilities will be discussed in section 3. For practical purposes, however, all the α_o' may be rendered discrete by placing the system in a box,* so that a single normalization condition can be imposed on all basic vectors uniformly throughout the discussion:

$$\langle \alpha_o'' | \alpha_o' \rangle = \delta(\alpha_o'', \alpha_o') = \begin{cases} 1 & \text{if } \alpha_o^{i\,\prime\prime} = \alpha_o^{i\,\prime} \text{ for all } i \\ 0 & \text{otherwise.} \end{cases} \tag{1.35}$$

H_o is an operator function of the α_o, since the latter, being constants of the motion, commute with H_o. Hence

$$H_o |\alpha_o'\rangle = H_o' |\alpha_o'\rangle \tag{1.36}$$

---

* It is most convenient to assume that the box does not actually contain the system in the sense of providing an infinite potential barrier, but that it merely imposes periodic boundary conditions on the wave functions.

where the energy level H_o' of the state $|\alpha_o'\rangle$ is the corresponding ordinary function of the α_o'. It is sometimes convenient to choose H_o as one of the α_o.

When H_o is time independent the solution of Eq. (1.25) is immediately written down:

$$U_o(t'', t') = e^{-i H_o(t'' - t')} . \tag{1.37}$$

Hence

$$\bar{F}(t) = e^{i H_o t} F(t) e^{-i H_o t} , \tag{1.38}$$

$$|\bar{\psi}(t)\rangle = e^{i H_o t} |\psi(t)\rangle , \tag{1.39}$$

$$\bar{U}(t'', t') = e^{i H_o t''} U(t'', t') e^{-i H_o t'} . \tag{1.40}$$

Transition probabilities.

The operators α_o and H_o remain invariant under the transformation to the interaction representation:

$$\bar{\alpha}_o = \alpha_o , \qquad \bar{H}_o = H_o . \tag{1.41}$$

As a consequence, transition probabilities taken between members of the basic states $|\alpha_o'\rangle$ of the "reference system" can be expressed equally well in terms of either the Schrödinger or the interaction transformation operators. If the actual system H is known to be in the Schrödinger state $|\alpha_o'\rangle$ at the time t' then the probability of finding it in the Schrödinger state $|\alpha_o''\rangle$ at the time t'' is

$$P(\alpha_o'', t'' | \alpha_o' \; t') = \left| \langle \alpha_o'' | \; U(t'', t') | \alpha_o' \rangle \right|^2$$

$$= \left| e^{-i H_o'' t'' + i H_o' t'} \langle \alpha_o'' | \bar{U}(t'', t') | \alpha_o' \rangle \right|^2$$

$$= \left| \langle \alpha_o'' | \; \bar{U}(t'', t') | \alpha_o' \rangle \right|^2 . \tag{1.42}$$

Transition probabilities are often computed approximately by inserting the first term or two of the expansion (1.31a) into (1.42).

This section may be closed with the observation that the Schrödinger and interaction representations have been defined so as to coalesce with the Heisenberg representation at $t = 0$:

$$|\bar{\psi}(0)\rangle = |\psi(0)\rangle = |\underset{\sim}{\psi}\rangle . \tag{1.43}$$

The formalism above would not have been significantly altered if other arbitrary meeting points t_o had been selected, but no real generality would have been gained thereby since the system can always be displaced in time without altering its essential physical characteristics.

2. GREEN'S FUNCTIONS AND FOURIER TRANSFORMS

Temporal switching operators.

It is often a useful mathematical device to "switch on" a quantum state abruptly. The operators which perform this action for the systems H_o and H are respectively

$$G_{o\pm}(t'', t') = \mp i\, e^{\mp\epsilon(t'' - t')}\, \theta_\pm(t'' - t')\, U_o(t'', t') , \tag{2.1}$$

$$G_\pm(t'', t') = \mp i\, e^{\mp\epsilon(t'' - t')}\, \theta_\pm(t'' - t')\, U(t'', t') . \tag{2.2}$$

Actually, the $+$ operators switch a state on and the $-$ operators switch it off. The exponential factors damp the state in the future or the past as the case may be. They are inserted here so as to make certain future limiting procedures convergent. ϵ is a small positive number, having the dimensions of energy, which will eventually tend to zero.

Switching operators are Green's functions.

The following properties of the $\theta_\pm$ functions will be needed:

$$\frac{d}{dt}\theta_\pm(t) = \pm\delta(t) , \tag{2.3}$$

$$\theta_\pm(-t) = \theta_\mp(t) , \tag{2.4}$$

$$\theta_+(t) + \theta_-(t) = 1 . \tag{2.5}$$

Using (2.3) and the differential equations satisfied by the operators U_o, U, one finds

$$\left[i\,\partial/\partial t'' - H_o(t'') \pm i\epsilon \right] G_{o\pm}(t'', t') = \delta(t'' - t'), \tag{2.6}$$

$$\left[i\,\partial/\partial t'' - H(t'') \pm i\epsilon \right] G_{\pm}(t'', t') = \delta(t'' - t') . \tag{2.7}$$

Eqs. (2.6) and (2.7) entitle $G_{o\pm}$ and $G_{\pm}$ to be called the Green's functions of the systems H_o and H respectively. The language of Green's functions allows one to reformulate the perturbation problem in terms of an integral equation which directly connects one system with the other:

$$G_{\pm}(t'', t') = G_{o\pm}(t'', t') + \int_{-\infty}^{\infty} G_{o\pm}(t'', t''') H_1(t''') G_{\pm}(t''', t')dt''' . \tag{2.8}$$

<u>Fourier transforms.</u>

If neither H_o nor H has any explicit dependence on t, then

$$U_o(t'', t') = e^{-i H_o(t'' - t')} , \qquad U(t'', t') = e^{-i H(t'' - t')} ; \tag{2.9}$$

and the functions $G_{o\pm}$ and $G_{\pm}$ depend only on the difference between the times t'' and t'. Setting $t' = 0$, one has

$$G_{o\pm}(t, 0) = \mp i\, \theta_{\pm}(t)\, e^{-i\,(H_o \mp i\epsilon)t} \tag{2.10}$$

$$G_{\pm}(t, 0) = \mp i\, \theta_{\pm}(t)\, e^{-i\,(H \mp i\epsilon)t} . \tag{2.11}$$

With $G_{o\pm}$, $G_{\pm}$ depending only one one variable it is useful to take their Fourier transforms.

$$G_{o\pm}(E) \equiv \int_{-\infty}^{\infty} G_{o\pm}(t, 0)\, e^{iEt}\, dt = \frac{1}{E - H_o \pm i\epsilon}, \tag{2.12}$$

$$G_{\pm}(E) \equiv \int_{-\infty}^{\infty} G_{\pm}(t, 0)\, e^{iEt}\, dt = \frac{1}{E - H \pm i\epsilon}. \tag{2.13}$$

As long as ϵ remains finite $G_{o\pm}(E)$, $G_{\pm}(E)$ are not singular for real E.

Algebraic relations.

With the use of the operator identity

$$(A + B)^{-1} \equiv A^{-1}\left[1 - B(A + B)^{-1}\right] \equiv \left[1 - (A + B)^{-1} B\right] A^{-1} \tag{2.14}$$

$G_{\pm}(E)$ may be expressed in terms of $G_{o\pm}(E)$ as follows.

$$G_{\pm}(E) = G_{o\pm}(E)\left[1 + H_1 G_{\pm}(E)\right] \tag{2.15a}$$

$$= \left[1 + G_{\pm}(E)\, H_1\right] G_{o\pm}(E) . \tag{2.15b}$$

Eq. (2.15a) is simply the Fourier transform of the integral equation (2.8). It is customary to refer to Eqs. (2.15) also as integral equations. This is because in order to deal with them analytically it is necessary to express them in matrix form, in which case integrations over matrix elements generally make their appearance. It is noteworthy, however, that the Fourier transformation has made the equations of interest more compact than before.

Eqs. (2.15) can be solved formally to give

$$G_{\pm}(E) = \left[1 - G_{o\pm}(E)\, H_1\right]^{-1} G_{o\pm}(E) \tag{2.16a}$$

$$= G_{o\pm}(E)\left[1 - H_1\, G_{o\pm}(E)\right]^{-1} . \tag{2.16b}$$

"Approximate" solutions are obtained by taking the first few terms of a binomial expansion of these expressions. Obviously, difficult questions of convergence are involved here.

Time independence.

The time independence of H_0 and H will be assumed throughout the remainder of this article unless otherwise indicated. Then the system H, like H_0, has N independent commuting constants of motion α^i, which remain invariant under a transformation to the Heisenberg representation.

$$\underset{\sim}{\alpha} = \alpha \qquad\qquad \underset{\sim}{H} = H \quad . \tag{2.17}$$

Introducing basic vectors corresponding to these constants, one may write

$$\alpha|\alpha'\rangle = \alpha'|\alpha'\rangle , \qquad H|\alpha'\rangle = H'|\alpha'\rangle \quad , \tag{2.18}$$

$$\langle\alpha''|\alpha'\rangle = \delta(\alpha'', \alpha'). \tag{2.19}$$

A central task of succeeding sections will be to set up a correspondence between the vectors $|\alpha'\rangle$ and the vectors $|\alpha_0'\rangle$ and to express the former in terms of the latter. The operator $\bar{U}(t'', t')$, which now has the form

$$\bar{U}(t'', t') = e^{i H_0 t''} e^{-i H(t'' - t')} e^{-i H_0 t'} , \tag{2.20}$$

turns out to be of great importance in this undertaking.

3. TYPES OF SYSTEMS

Classification of states.

The states $|\alpha'\rangle$ of a system H may be classified into bound, mixed, and free states. For example, if the system has a classical analog one may introduce the coordinates q^i, place the system in a rectangular box of side L, construct, in the coordinate representation, an eigenfunction $\psi(q)$ which remains finite as $L \to \infty$, and define the corresponding state to be bound, mixed, or free according as the integral $\int \psi^* \psi \, d^N q$ is of order L^0, L^n, or L^N, where N is the number of degrees of freedom, $0 < n < N$, and $d^N q$ is the volume element in coordinate space. Related criteria may be employed for nonclassical systems.

Simple and complex systems.

If H possesses bound or mixed states than the ranges of value of some of the α' must include discrete sets even when the system is not placed in a box. If all the α' for a given state $|\alpha'\rangle$ come from discrete sets, the state is bound. The system will be called simple if $|\alpha'\rangle$ is free whenever at least one of the α' comes from a continuum. Otherwise it will be called complex. The states of a simple system are always either bound or free, never mixed.

A complex system is usually characterized as being composed of two or more simple subsystems. A mixed state is one in which some of the subsystems are in bound states while the others are in free states. The subsystems may interact with one another, but not strongly enough to destroy their individual identities. Otherwise a separation into simple subsystems becomes meaningless. Sometimes one separation may be used for one range of values of the α' while a different one must be used over another range.

In discussing the various situations which can arise it will be convenient to develop our notation by replacing the general labels α' by other labels which distinguish between free and bound states. For simple systems the Greek letter ζ will be reserved to denote free states and the capital J to denote bound states. Eqs. (2.18, 19) will then be replaced by

$$\zeta|\zeta'\rangle = \zeta'|\zeta'\rangle, \qquad J\,|J'\rangle = J'\,|J'\rangle, \tag{3.1}$$

$$\langle\zeta''|\zeta'\rangle = \delta(\zeta'',\zeta'), \quad \langle J''|J'\rangle = \delta(J'',J'), \qquad \langle\zeta''|J'\rangle = 0, \tag{3.2}$$

If the system has a classical analog the operators which J collectively denotes are usually chosen to be the quantum counterparts of the classical <u>action</u> variables. Some of these action variables may be included among the ζ, though not all; in the case of free states at least one of the J' must be replaced by a label referring to the continuous spectrum.

Mixed states of a complex system may be designated by expressions of the form $|\zeta_A', \zeta_B' \ldots, J_E', J_F' \ldots\rangle$, the labels ζ_A', ζ_B' ... referring to the free subsystems and the J_E', J_F' ... referring to the bound ones. However, the system of interest H is sometimes so complicated (as in the case of interacting fields) that the physical separation into subsystems is by no means obvious, so that the labels above may have a simple interpretation only with respect to the reference system H_o. This leads us directly to the next topic.

<u>Separable Hamiltonians.</u>

The subsystems of a complex system need not interact with one another, and if they do not the Hamiltonian operator is expressible as a

sum of terms, each corresponding to only one subsystem, and will be called separable. The separation may be more mathematical than physical. For example, for two particles interacting through central forces the relative coordinates form one simple subsystem and the coordinates of the center of mass another.

If system H is complex the Hamiltonian operator H_o of the reference system is usually chosen to be separable, the perturbation H_1 providing interaction between the simple subsystems. The labels used to specify the eigenvectors of H_o then usually have a simple physical interpretation.

A special example.

It is instructive to consider a special example of a complex system which illustrates some of the important situations occurring in practice, and for which several different reference systems must be chosen depending on circumstances.*

Let a particle B be attracted by a center of force C, the interaction potential being H_1. Let a particle A simultaneously interact with B through a potential H_2. (Here, instead of one perturbation we have two; in the preceding discussion they have been regarded as lumped together.) The total Hamiltonian operator for this system is

$$H = H_o + H_1 + H_2 \tag{3.3}$$

where

$$H_o = H_A + H_B \quad , \tag{3.4}$$

---

* This system is discussed in greater detail in section 12.

H_A and H_B being the kinetic energies of particles A and B. It is convenient to write also

$$H_o = H_R + H_T \tag{3.3}$$

where H_R is the rotational and H_T the translational energy of the pair AB.

Consider a scattering situation in which the initial state finds particle B bound in an orbit around C, with A coming in from infinity to collide with B. (See Fig. 1.) This state may be described by labels ζ_A' referring to the free motion of A, and J_{BC}' referring to the bound condition of B to C. For this state the convenient Hamiltonian operator to introduce for the reference system is $H_o + H_1$, which separates into H_A and $H_B + H_1$. The perturbation operator is then H_2. The state vector $|\zeta_A', J_{BC}'\rangle$ will sometimes also be denoted by $|\alpha_{01}'\rangle$, the subscripts 0 and 1 on the α's indicating that the Hamiltonian operator of the reference system, which may be called the "unperturbed Hamiltonian," is the sum of H_o and H_1.

The initial state $|\zeta_A', J_{BC}'\rangle$ can lead to several types of final states, as pictured in Figs. 2 to 5. Fig. 2 shows a final state which is of the same type as the initial state, with merely new values ζ_A'', J_{BC}'', α_{01}'' for the labels.

In Fig. 3 particle B has been knocked loose from its bond with C so that both A and B are free. This final state may be denoted by labels ζ_A'', ζ_B'', or collectively α_0'', the convenient unperturbed Hamiltonian being simply H_o, which separates according to Eq. (3.4). In this case the perturbation is $H_1 + H_2$.

Fig. 4 shows a "pick-up" process in which particle B loses its bond with C and becomes bound with A instead. The convenient unperturbed Hamiltonian here is $H_0 + H_2$, which separates into H_T and $H_R + H_2$, and the perturbation is H_1. Suitable labels for this final state are $\mathcal{J}_T''$, J_R'' (referring to the free translational motion and bound rotational motion of the pair AB) or collectively α_{02}''. The inverse of this particular reaction is a "stripping" process, which is also of interest.

Fig. 5 shows the remaining possibility, a capture process in which A, B and C become all bound together. There is no obvious reference system for this state; the total Hamiltonian operator H must be examined more or less directly. Suitable labels for the state would be J'' or α'', referring to the total system. We shall see later that such a state is actually not a possible final state for the reaction unless some other physical process, such as radiation, takes place; that such a state would, in fact, be metastable even if it "existed" for any length of time at all.

The reader may easily construct more complicated examples, for instance by adding a third potential H_3 acting between A and C, and considering the final state in which A is bound to C while B is free. It is sufficiently clear from the present example, however, how the reference system would be chosen under almost any circumstance, of the same general types, which may arise.

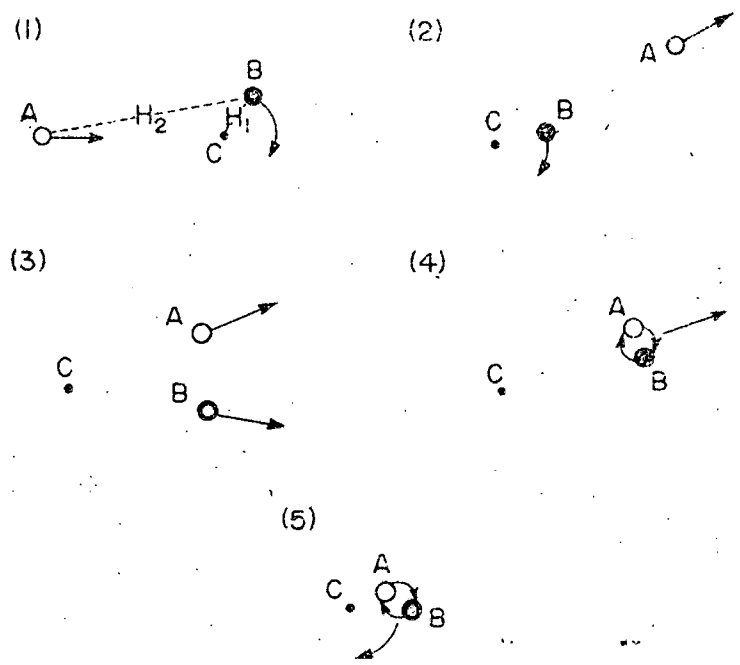

FIG. 1 AN INITIAL CONFIGURATION FOR A TWO PARTICLE SYSTEM

FIGS. 2 TO 5
POSSIBLE FINAL CONFIGURATIONS

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The basic spectral types.

The precise form which perturbation theory must take in order to describe the behavior of a given physical system H depends on the structure of the spectrum of H in the energy range of interest and also on the structure of the spectrum of the most convenient reference system H_0. For simple systems three basic spectral types may be distinguished:

1. The simplest type of spectrum is the one which occurs when H and H_0 each possess only discrete bound states for which a one-to-one correspondence can be set up. An example of this situation is pictured in Fig. 6 in which the correspondence is indicated schematically by dotted lines connecting the levels. There will in general be a shift in the positions of the energy levels in passing from system H_0 to system H. The occurrence of possible degeneracies is not pictures in the figure.

2. The second basic spectral type is one which occurs when H and H_0 possess free states as well as bound, the discrete energy levels of the bound states in each case lying below the continuum levels of the free states. In the typical situation the free states can be put into one-to-one correspondence but suffer no level shift in passing from one system to the other. The bound states, on the other hand, will generally have levels shifted relative to one another as in spectral type 1, and may not necessarily be able to be put into one-to-one correspondence owing to the fact that one system may have more bound states than the other. Such a situation is pictured in Fig. 7 in which system H has bound states which have no counterparts in H_0. This spectral type is typically encountered in simple scattering problems and will be dealt with in sections 4 and 7. The situations in which one or both of the systems has no bound states may be regarded as special cases of it.

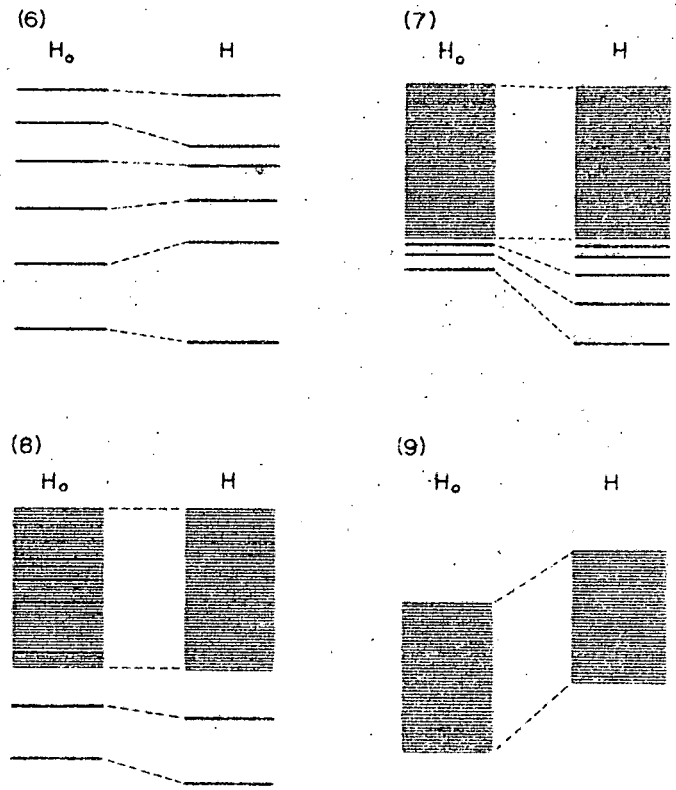

FIG.6 BOUND STATE LEVEL DIAGRAM

FIG.7 A LEVEL DIAGRAM FOR SIMPLE SCATTERING PROBLEMS

FIG.8 A TYPICAL LEVEL DIAGRAM FOR DECAYING SYSTEMS

FIG.9 THE TYPICAL SITUATION IN QUANTUM FIELD THEORIES

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3. In the third basic spectral type H and H_0 again possess both bound and free states. The important point, however, is that the energy levels of some of the bound states of the reference system H_0 fall within the range of the continuum levels of its free states. These bound states generally have no counterparts in the actual system H. The switching on of the perturbation H_1 annihilates them except in trivial cases in which there is no coupling between the bound and free states. Situations of this kind arise in the study of decaying systems and will be treated in section 11. The states of H_0 which have no counterparts in H are those which in physical reality undergo decay.

The energy spectra of complex systems will generally combine the features of the three simple basic types. This is evident, for example, in the case of the special complex system pictured in Figs. 1 to 5. The combination of basic-type features may not, however, necessarily result from simple additivity of the subsystem spectra. This is especially true of complex decaying systems, which may possess spectra of type 3 as an intrinsic result of their complex character combined with special properties of the interaction H_1. In fact, when spectral type 3 occurs for simple systems the reference system H_0 usually has some rather artificial properties which arise out of the peculiar way in which a decay problem poses itself.

The existence of situations involving decay is responsible for our previous remark that the state pictured in Fig. 5 could not actually be a possible final state for the collision process starting in Fig. 1. Energy must be conserved in a collision, and a discrete energy level of a bound state (Fig. 5) would therefore exist lying within a set of continuum levels (Figs. 1 to 4). The bound state of Fig. 5 could be stable at the energy in question only if a barrier were placed around the system. The

removal of this barrier would be a perturbation annihilating the state.

We must finally mention the important situation pictured in Fig. 9 in which H has free states whose continuum levels are shifted relative to those of H_0. This situation is not counted among the basic spectral types since it occurs non-trivially only in connection with complex systems, specifically in quantum field theories. It can occur in combination with any or all of the basic spectral types and has historically been very troublesome. It will be dealt with in section 10.

4. SIMPLE SCATTERING

Confined forces.

The theory of scattering provides perhaps the most natural point of entry into the further mathematical development of the operator formalism. For definiteness consider a system H consisting of a single particle interacting with a fixed scatterer. The force exerted by the scatterer need not be centrally directed nor even velocity independent. However, it may be necessary to choose the reference system H_0 so as to include part of this force, for it will be assumed that the remaining force is confined to a limited region of space called the scattering region. If the force is attractive the energy spectra of systems H_0 and H may have the structures shown in Fig. 7, although, in general, bound states may be absent in either or both of the two. In any case bound states will be ignored for the present.

Retarded waves.

The scattering problem is solved if the free-state eigenvectors of H are known. In analogy with the wave theories of light, sound, etc. one may write these eigenvectors in the form

$$|\zeta_+'\rangle \sim |\zeta_0'\rangle + |\mathrm{ret}'\rangle \tag{4.1}$$

where $|\mathrm{ret}'\rangle$ represents a retarded wave and $|\zeta_0'\rangle$ is a free-state eigenvector of H_0 suitable for representing the incoming particle (e.g. incident plane wave, or spherical wave of given angular momentum). Eq. (4.1) presupposes at once a natural one-to-one correspondence between the free states $|\zeta_0'\rangle$ of H_0 and the free states $|\zeta_+'\rangle$ of H. The significance of the + sign on the ζ_+' will become clearer in

subsequent paragraphs and is connected with the fact that a scattering process introduces a preferred (in this case positive) direction in time into the scheme of things.

Eq. (4.1) is supposed to be an asymptotic equation and should more properly be written in the form

$$\langle q'' | \zeta_+' \rangle \sim \langle q'' | \zeta_0' \rangle + \langle q'' | \mathrm{ret}' \rangle \tag{4.2}$$

where the q'' are the coordinates of the particle and the asymptotic region is that at large distances from the scatterer. However, no misunderstanding will arise if the coordinate eigenvectors $|q''\rangle$ are frequently dropped.

The writing of (4.1) as an asymptotic equation is sufficient for present purposes since a complete knowledge of the eigenvectors $|\zeta_+'\rangle$ is not actually necessary for the solution of the scattering problem. Only the asymptotic behavior of the corresponding wave functions is needed.

Wave packets.

The scattering process is more graphically represented if one constructs a wave packet:

$$|\underset{\sim}{\psi}\rangle = \sum{}' f(\zeta_0') |\zeta_+'\rangle . \tag{4.3}$$

where $f(\zeta_0')$ is a (generally complex) function which is "peaked" around a particular set of values of the ζ_0', and where the symbol $\sum'$ denotes a summation over all of the dashed variables. The wave packet may itself be separated into an incoming part and a retarded wave.

$$|\underset{\sim}{\psi}\rangle \sim |\text{in}\rangle + |\text{ret}\rangle , \tag{4.4}$$

$$|\text{in}\rangle = \sum{}' f(\zeta_o{}')|\zeta_o{}'\rangle , \tag{4.5}$$

$$|\text{ret}\rangle = \sum{}' f(\zeta_o{}')|\text{ret}'\rangle . \tag{4.6}$$

The vector $|\underset{\sim}{\psi}\rangle$ is a constant Heisenberg state vector. To picture the moving packet one must pass to the Schrödinger representation. With the help of (1.20), (1.43) and (2.9) one gets

$$|\psi(t)\rangle = e^{-i\,Ht}|\underset{\sim}{\psi}\rangle = \sum{}' e^{-i\,H't} f(\zeta_o{}')|\zeta_+{}'\rangle . \tag{4.7}$$

The complex phase of the function f must, of course, be selected in such a way that the packet moves in a physically interesting fashion. Here it is necessary to rely on a previous knowledge of the behavior of wave packets, based on more precise details of the structure of a given Hamiltonian H (or H_o) than can be got from the abstract operator formalism alone. The packet must be formed in such a way that for large negative and positive values of t it is found at a large distance from the scattering region. Under these circumstances only the asymptotic parts of the energy eigenfunctions contribute significantly to the wave packet, and (4.7) may be replaced by

$$|\psi(t)\rangle \xrightarrow[t\to\pm\infty]{} \sum{}' e^{-i\,H't} f(\zeta_o{}')(|\zeta_o{}'\rangle + |\text{ret}'\rangle) . \tag{4.8}$$

For large $|t|$ both (4.7) and (4.8) provide a mutual cancellation of eigenwave amplitudes in and near the scattering region, although the precise manner in which this cancellation comes about is different in the two cases.

Definition of $|\mathrm{ret}'\rangle$.

So far the vector $|\mathrm{ret}'\rangle$ has not been well defined since an infinity of different functions $\langle q'' | \mathrm{ret}'\rangle$ can be chosen, all having the same asymptotic behavior. The most practically convenient choice is one which makes Eq. (4.1) exact, rather than merely asymptotic, outside of the scattering region:

$$\langle q'' | \zeta_+' \rangle = \langle q'' | \zeta_o' \rangle + \langle q'' | \mathrm{ret}' \rangle \quad \text{for } q'' \text{ outside scattering region.} \tag{4.9}$$

For then, since $\langle q'' | \zeta_+' \rangle$ satisfies the Schrödinger equation of the reference system outside of the scattering region, so also will $\langle q'' | \mathrm{ret}' \rangle$. Indeed, $\langle q'' | \mathrm{ret}' \rangle$ may be allowed to satisfy this equation <u>everywhere</u> except at a single point within the scattering region, which may be called the <u>origin</u>:

$$(H_o - H')\,|\mathrm{ret}'\rangle = |\delta'\rangle \tag{4.10}$$

where

$$\langle q'' | \delta' \rangle = 0 \quad \text{except when } q'' \text{ is the origin.} \tag{4.11}$$

The function $\langle q'' | \mathrm{ret}' \rangle$ then has a simple structure in terms of known functions which provide an analytical apparatus independent of the size of the scattering region and which can therefore be applied to a wide variety of problems.

Eq. (4.10) has, in general, two independent solutions. It is necessary to choose the linear combination of these solutions which satisfies the boundary condition appropriate to scattering in the positive time direction. This boundary condition may be expressed in a form which

makes use of the wave packet picture, namely

$$\sum{}' \, e^{-i H' t} f(\zeta_0') \, | \, \mathrm{ret}' \rangle \xrightarrow[t \to -\infty]{} 0 \quad . \tag{4.12}$$

That is, the retarded (or scattered) wave disappears as t tends to $-\infty$. In fact it gets sucked into the origin upon time reversal; or conversely, it emerges from the origin as a scattered packet as time passes from $-\infty$ to ∞. The vectors $|\delta'\rangle$ may be regarded as the <u>sources</u> or <u>sinks</u> of this packet.

<u>Advanced waves.</u>

The other independent solution of Eq. (4.10) corresponds to an <u>advanced</u> wave, satisfying the conditions

$$(H_0 - H') \, | \, \mathrm{adv}' \rangle = | \, \delta' \rangle , \tag{4.13}$$

$$\sum{}' \, e^{-i H' t} f(\zeta_0') \, | \, \mathrm{adv}' \rangle \xrightarrow[t \to \infty]{} 0 \quad . \tag{4.14}$$

The advanced wave is annihilated with the passage of time.

For the correlation of actual experimental results with the results of the theory of scattering the use of wave packets as above is absolutely necessary. (See further section 8.) Eqs. (4.12) and (4.14), expressing boundary conditions, are crucial. It should be observed that these equations require the retarded and advanced waves to be <u>completely</u> sucked into the origin as t tends to $-\infty$ and $+\infty$ respectively. This

obviously requires the use of finite packets.*

In analogy with the definition of the "radiation field" in electrodynamics [14] and acoustics, one may define vectors

$$|\mathrm{rad}'\rangle \equiv |\mathrm{ret}'\rangle - |\mathrm{adv}'\rangle \tag{4.15}$$

satisfying

$$(H_o - H')\,|\mathrm{rad}'\rangle = 0 \,. \tag{4.16}$$

Eqs. (4.8), (4.12) and (4.14) then yield

$$|\psi(t)\rangle \xrightarrow[t \to -\infty]{} \sum{}' \, e^{-i H' t} f(\zeta_o')\,|\zeta_o'\rangle \,, \tag{4.17}$$

$$|\psi(t)\rangle \xrightarrow[t \to \infty]{} \sum{}' \, e^{-i H' t} f(\zeta_o')\,(|\zeta_o'\rangle + |\mathrm{rad}'\rangle) \,. \tag{4.18}$$

The scattering operator.

At this point is is convenient to return briefly to the Heisenberg representation and Eq. (4.4). Instead of separating the packet into incoming and retarded waves, one may also separate it into outgoing and advanced waves:

$$|\underset{\sim}{\psi}\rangle \sim |\mathrm{out}\rangle + |\mathrm{adv}\rangle \tag{4.19}$$

---

* There is a slight difficulty here, connected in the nonrelativistic case with the fact that a truly finite packet tends to spread infinitely fast, and in the relativistic case with the fact that a complete set of eigenfunctions is not available with which to construct such packets if only positive energy particle states are allowed. (Cf. van Kampen, reference [203].) A more detailed study (e.g. Low, reference [16]) shows, nevertheless, that Eqs. (4.12) and (4.14) are essentially correct.

where

$$|\mathrm{adv}\rangle = \sum{}' f(\zeta_0{}')\,|\mathrm{adv}'\rangle , \tag{4.20}$$

$$|\mathrm{out}\rangle = |\mathrm{in}\rangle + |\mathrm{rad}\rangle , \tag{4.21}$$

$$|\mathrm{rad}\rangle = |\mathrm{ret}\rangle - |\mathrm{adv}\rangle = \sum{}' f(\zeta_0{}')\,|\mathrm{rad}'\rangle . \tag{4.22}$$

Heisenberg [19] has introduced an operator S called the <u>scattering operator</u> which is defined by the equation

$$|\mathrm{out}\rangle = S\,|\mathrm{in}\rangle \qquad \text{for all packets.} \tag{4.23}$$

In the limit of a very broad packet (which is equivalent to a very peaked function $f(\zeta_0{}')$) one has $|\mathrm{in}\rangle \rightarrow |\zeta_0{}'\rangle$, $|\mathrm{rad}\rangle \rightarrow |\mathrm{rad}'\rangle$, and evidently

$$\langle \zeta_0{}''|\,S\,|\zeta_0{}'\rangle = \delta(\zeta_0{}'',\zeta_0{}') + \langle \zeta_0{}''|\,\mathrm{rad}'\rangle . \tag{4.24}$$

In its matrix form the scattering operator is known as the <u>S-matrix</u>. The S-matrix is determined completely by the asymptotic behavior of the time independent Heisenberg eigenfunctions of the Hamiltonian operator H. A knowledge of the S-matrix completely solves the scattering problem.

The S-matrix may be related to the transformation operator in the interaction representation, through which its explicit construction may be achieved. Here it is necessary to assume

$$H_0{}' = H' , \tag{4.25}$$

i.e. that the energy levels undergo <u>no shift</u> in the passage from H_0 to H. Eq. (4.25) is automatically satisfied for the simple scattering problems with confined forces presently under consideration, the energy being simply the kinetic energy of the particle at large distances from the scattering

region and being therefore common to both systems H and H_o. For other systems to be considered later, however, it will be necessary to take care in making this assumption.

Eq. (1.39) gives the transformation to the interaction representation. Applying it to Eqs. (4.17, 18) and using (4.25), one gets

$$\left|\bar{\psi}(-\infty)\right\rangle = \sum{}' f(\zeta_o{}')\left|\zeta_o{}'\right\rangle = \left|\text{in}\right\rangle , \tag{4.26}$$

$$\left|\bar{\psi}(\infty)\right\rangle = \sum{}' f(\zeta_o{}')\left(\left|\zeta_o{}'\right\rangle + \left|\text{rad}'\right\rangle\right) = \left|\text{out}\right\rangle . \tag{4.27}$$

Evidently

$$S = \bar{U}(\infty, -\infty) . \tag{4.28}$$

Thus the transformation operator in the interaction representation contains full information on the behavior of the free-state eigenfunctions of H in the asymptotic region. It also contains complete information on their behavior everywhere else as well. For, remembering that all representations coalesce at $t = 0$ (Eq. (1.43)), one may write

$$\left|\underset{\sim}{\psi}\right\rangle = \bar{U}(0, -\infty)\left|\bar{\psi}(-\infty)\right\rangle = \bar{U}(0, -\infty)\left|\text{in}\right\rangle . \tag{4.29}$$

In the limit of a very broad packet one has $\left|\text{in}\right\rangle \longrightarrow \left|\zeta_o{}'\right\rangle$ and $\left|\underset{\sim}{\psi}\right\rangle \longrightarrow \left|\zeta_+{}'\right\rangle$. Hence

$$\left|\zeta_+{}'\right\rangle = \bar{U}(0, -\infty)\left|\zeta_o{}'\right\rangle . \tag{4.30}$$

5. LIMITING PROCEDURES

Adiabatic switching.

Eq. (4.30) expresses the free-state eigenvectors of the system H directly in terms of those of the reference system H_o and points the way toward their explicit construction. However, the problem is immediately encountered of how to give a proper definition to expressions of the form $\bar{U}(0, \mp\infty)$ and $\bar{U}(\pm\infty, \mp\infty)$, which is certainly not clear from Eq. (2.20). A key to this problem is supplied by Eqs. (4.17, 18) which state that for large values of $|t|$ the wave packet satisfies the Schrödinger equation of the unperturbed reference system. (Remember the $|\mathrm{rad}^{\mp}\rangle$ are eigenvectors of H_o by Eq. (4.16).) As long as the packet is at a large distance from the scattering region it matters very little whether the perturbation H_1 is present or not. This suggests the use of the widely employed mathematical device of switching the perturbation on as the packet approaches the scattering region and off again after it has been scattered, in order to give a precise definition to the limiting procedure implied by the symbols $t \longrightarrow \pm\infty$.

In order to accommodate the widest variety of packet sizes and shapes the switching process should be very gradual, i.e. adiabatic. There are an infinity of modes of accomplishing adiabatic switching, but the one which is probably the simplest analytically is that which replaces H_1 by

$$H_1^{ad}(t) = e^{-\epsilon|t|} H_1 , \qquad \epsilon \longrightarrow +0 . \tag{5.1}$$

The time of duration of the perturbation under the adiabatic switching procedure may be defined as

$$\int_{-\infty}^{\infty} H_1^{ad}(t)\, dt/H_1 = 2/\epsilon \quad . \tag{5.2}$$

Passing to the interaction representation (Eq. (1.38)), one gets

$$\bar{H}_1^{ad}(t) = e^{i H_o t} H_1 e^{-i H_o t - \epsilon |t|} \quad . \tag{5.3}$$

This equation may be substituted directly into Eqs. (1.31a), (1.32a) to get explicit expressions for the interaction transformation operator $\bar{U}^{ad}(t'', t')$ under the adiabatic process (5.1). It is convenient to make the following transformation of variables:

$$\begin{aligned} t_1' &= t_1 , & t_1 &= t_1' , \\ t_2' &= t_2 - t_1 , & t_2 &= t_1' + t_2' , \\ &\cdots\cdots & &\cdots\cdots \\ t_n' &= t_n - t_{n-1} , & t_n &= t_1' + t_2' \ldots + t_n' . \end{aligned} \tag{5.4}$$

Then one gets for the operators $\bar{U}^{ad}(t, \mp\infty)$, where t is positive or negative according as the ∞ carries a $+$ or $-$ sign, [40]

$$\bar{U}^{ad}(t,\mp\infty) = 1+\sum_{n=1}^{\infty}(\mp i)^n \int_{-\infty}^{\infty} dt_1' \ldots \int_{-\infty}^{\infty} dt_n' \; \theta_{\mp}(t_1'-t)\; \theta_{\mp}(t_2')\ldots\theta_{\mp}(t_n')$$

$$e^{i H_0 t_1' \pm n\epsilon t_1'} H_1 \ldots e^{i H_0 t_n' \pm \epsilon t_n'} H_1 \; e^{-i H_0(t_1'+\ldots+t_n')}$$

$$= 1+\sum{}' \sum_{n=1}^{\infty}(i)^n \int_{t}^{\mp\infty} dt_1' \ldots \int_{0}^{\mp\infty} dt_n' \; e^{-i(E'-H_0\pm i\, n\epsilon)t_1'} H_1 \ldots$$

$$\ldots e^{-i(E'-H_0\pm i\epsilon)t_n'} H_1 \left|\alpha_0'\right\rangle\left\langle\alpha_0'\right|$$

$$= e^{i H_0 t}\left[1+\sum{}' \sum_{n=1}^{\infty} \frac{1}{E'-H_0\pm in\epsilon} H_1^{ad}(t) \ldots\right.$$

$$\left.\ldots \frac{1}{E'-H_0\pm i\epsilon} H_1^{ad}(t)\left|\alpha_0'\right\rangle\left\langle\alpha_0'\right|\right] e^{-i H_0 t} , \tag{5.5}$$

where $E' = H_0'$. The second form is obtained through multiplication on the right by the equation

$$1 = \sum{}' \left|\alpha_0'\right\rangle\left\langle\alpha_0'\right| \tag{5.6}$$

which expresses the completeness condition for the basic vectors of the reference system.

Scattering will be properly described if we now define

$$\bar{U}(t,\mp\infty) \equiv \lim_{\epsilon\to 0} \bar{U}^{ad}(t,\mp\infty) , \tag{5.7}$$

$$\bar{U}(\pm\infty,\mp\infty) \equiv \bar{U}(0,\pm\infty)^{*}\, \bar{U}(0,\mp\infty), \tag{5.8}$$

whenever the limit (5.7) exists.

Convergence of the series (5.5).

Postponing the question of the existence of the limit (5.7), we shall first say something about the convergence of the series (5.5). Little generality is lost if t is set equal to zero so that

$$\bar{U}^{ad}(0, \mp\infty) = \sum{}' u_{\pm}(\alpha_0') , \tag{5.9}$$

$$u_{\pm}(\alpha_0') = \sum_{n=0}^{\infty} u_{n\pm}(\alpha_0') , \tag{5.10}$$

$$u_{0\pm}(\alpha_0') = |\alpha_0'\rangle\langle\alpha_0'| , \tag{5.11}$$

$$u_{n\pm}(\alpha_0') = r_{n\pm}(E') \, u_{n-1\pm}(\alpha_0') , \qquad n \geqslant 1 , \tag{5.12}$$

$$r_{n\pm}(E') = (E' - H_0 \pm i\, n\epsilon)^{-1} H_1 . \tag{5.13}$$

Since H_0 is an Hermitian operator the following inequality holds:

$$|E' - H_0 \pm i\, n\epsilon| \geqslant n\epsilon . \tag{5.14}$$

Therefore, by the ratio test of analysis one can assert that the series (5.10) is absolutely convergent as long as ϵ remains finite. For, the "ratio" of successive terms is given by expression (5.13), and

$$\lim_{n \to \infty} r_{n\pm}(E') = 0 . \tag{5.15}$$

Strictly speaking, more rigor is required here. Eq. (5.15) is valid only if, for finite n and ϵ, $r_{n\pm}(E')$ is a bounded operator, i.e. if all its eigenvalues are finite.* In bound-state problems, and in simple scattering problems with forces of finite range, this is generally the case. However, in so-called "local" field theories $r_{n\pm}(E')$ is unbounded, the trouble arising from the high energy matrix elements of H_1. Conventional practice has therefore been to impose an artificial high energy "cut-off" on the matrix elements, then to carry out certain "renormalization" procedures (see section 10), and finally to allow the cut-off to become infinite. (Even when the cut-off is never explicitly mentioned this is what present renormalization techniques amount to.) With the understanding that such procedures are to be adopted if necessary, one may regard $\bar{U}^{ad}(0, \mp\infty)$ as well defined by expansion (5.10).

Passage to the limit $\epsilon \to 0$.

Difficulties now arise, however, in the passage to the limit $\epsilon \to 0$. Although the operators $\bar{U}^{ad}(t, \mp\infty)$ are well-defined for finite ϵ their matrix elements may nevertheless not have well defined limits. For example, these limits will later be seen generally not to exist for bound state matrix elements or, in the case of complex systems, mixed state matrix elements. Moreover, these limits may not even exist for all the free state matrix elements of simple systems, with which we are primarily concerned at the moment. We shall attempt to deal with these difficulties in the remainder of this

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* If the eigenvectors of $r_{n\pm}(E')$ do not form a complete set, $r_{n\pm}(E')$ is said to be bounded if its norm is finite. (For the definition of "norm" see section 9.) Notice that we do not say that H_1 by itself must be bounded. For example, any potential which has even the weakest kind of singularity is unbounded, although $r_{n\pm}(E')$ may remain bounded.

section and in the next section, but it is here that the formal theory suffers most from lack of rigor.

In the limit of vanishing ϵ the mathematical role played by the imaginary parts of the denominators $E' - H_0 \pm i m\epsilon$ $(m = 1, 2 \ldots n)$ in expansion (5.5) reduces solely to one of determining the contour for integrations (if any occur) around the pole at E'. In this limit therefore the ratios $r_{n\pm}(E')$ may all be replaced by

$$r_{1\pm}(E') = G_{0\pm}(E')H_1 , \tag{5.16}$$

and one may write

$$\bar{U}(t, \mp\infty) = e^{i H_0 t} \bar{U}(0, \mp\infty) e^{-i H_0 t} , \tag{5.17}$$

where

$$\bar{U}(0, \mp\infty) = \sum{}' \sum_{n=0}^{\infty} \left[G_{0\pm}(E')H_1\right]^n |\alpha_0'\rangle\langle\alpha_0'| . \tag{5.18}$$

<u>Analytic continuation.</u>

The series (5.18) may be regarded as an expansion in powers of a "coupling constant" g to which the perturbation H_1 is imagined as being proportional:

$$H_1 = gV \equiv g(\partial H_1/\partial g) . \tag{5.19}$$

The free state matrix elements of series (5.18) are actually known [49] to possess finite radii of convergence in the complex g-plane for many simple scattering problems. Inside these radii, which generally vary from one matrix element to another, (5.18) defines operators $\bar{U}(0, \mp\infty)$ which are analytic in g. For these same problems, however, the transformation

operators from the eigenvectors of H_0 to the eigenvectors of H are known [46] to be analytic everywhere except at discrete sets of poles. Therefore (5.18) may be used to define $\bar{U}(0, \mp\infty)$ everywhere in the g-plane by analytic continuation. We may advertise this possibility by replacing (5.18) by its formal equivalent

$$\bar{U}(0, \mp\infty) = \sum{}' \left[1 - G_{0\pm}(E')H_1\right]^{-1} |\alpha_0'\rangle\langle\alpha_0'| \quad . \tag{5.20}$$

It will become apparent that this closed expression quite generally has meaning for all systems even when its expansion does not.*

<u>Alternative limiting procedure.</u>

Owing to the replacement (5.16), Eqs. (5.18) and (5.20) are not obtainable from an adiabatic switching of the perturbation as (5.5) is. They derive instead from a somewhat different limiting procedure. Using Eqs. (2.16a), (2.13), (2.11) and (2.20), one may write

$$\begin{aligned}\bar{U}(0, \mp\infty) &= \pm i\epsilon \sum{}' G_\pm(E') |\alpha_0'\rangle\langle\alpha_0'| \\ &= \pm i\epsilon \int_{-\infty}^{\infty} G_\pm(t, 0) e^{iH_0 t} dt \\ &= \epsilon \int_{-\infty}^{\infty} \theta_\mp(t') e^{\pm\epsilon t'} \bar{U}(0, t') dt' ,\end{aligned} \tag{5.21}$$

where $t' = -t$. Eqs. (5.18, 20, 21) therefore result from a convention which takes as the value of any bounded function $f(t)$ at $t = \pm\infty$ the expression [30]

$$f(\pm\infty) = \lim_{\epsilon \to +0} \epsilon \int_{-\infty}^{\infty} \theta_\pm(t) e^{\mp\epsilon t} f(t) dt \quad . \tag{5.22}$$

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* In some field theories there is evidence that the expansion is <u>nowhere</u> convergent. [115 to 122]

If $f(t)$ approaches a well defined limit as t becomes infinite then (5.22) gives that limit, as may be readily seen by a simple partial integration. However, (5.22) eliminates any part of $f(t)$ which oscillates like $e^{i\omega t}$ $(\omega \neq 0)$ as $t \to \pm\infty$. It will be seen in the next section that the operator $\bar{U}(0, t)$ frequently has such oscillating components. These components will therefore be eliminated by the definition (5.20, 21).

It is possible here to anticipate the fact that the operators $\bar{U}(0, \mp\infty)$ are often non-unitary. Although the operators $\bar{U}^{ad}(0, \mp\infty)$ are necessarily unitary by their construction, the operators $\bar{U}(0, \mp\infty)$ are, by (5.21), expressible only as weighted sums (<u>not</u> products) of unitary operators, which certainly does not guarantee their unitarity.

<u>Conventions to be adopted.</u>

The convention (5.22) is, for the remainder of this article, to be applied to the definition of the operators $\bar{U}(t, \mp\infty)$ and $\bar{U}(\pm\infty, t)$ as well as $\bar{U}(0, \mp\infty)$. Evidently then

$$\bar{U}(t, \mp\infty) = \bar{U}(t, 0)\, \bar{U}(0, \mp\infty) \tag{5.23}$$

$$= \bar{U}(\mp\infty, t)^{*}, \tag{5.24}$$

$$\bar{U}(\pm\infty, \mp\infty) = \bar{U}(\mp\infty, \pm\infty)^{*}. \tag{5.25}$$

From now on whenever expressions like (5.18, 20, 21) are written, involving the Green's functions $G_{0\pm}$ or $G_{\pm}$, it will always be understood that the limit $\epsilon \to 0$ is finally to be taken even though not explicitly indicated. With this understanding it is customary to write

$$\frac{E}{E^2 + \epsilon^2} = \mathcal{P}\,\frac{1}{E} , \tag{5.26}$$

$$\frac{1}{\pi}\,\frac{\epsilon}{E^2 + \epsilon^2} = \delta(E) , \tag{5.27}$$

$$G_{0\pm}(E') = \mathcal{P}\, 1/(E' - H_0) \mp \pi i\, \delta(E' - H_0) , \tag{5.28}$$

where the symbol $\mathcal{P}$ indicates that the principal value of any integral in which it appears is to be taken. Eq. (5.28), which separates the Green's function into its real and imaginary parts, makes explicit the effect of the contour integration around E'.

Eq. (5.27) may also be written in the form

$$\delta(E) = (2\pi)^{-1} \int_{-\infty}^{\infty} e^{i\,Et - \epsilon|t|}\, dt \xrightarrow[\epsilon \to 0]{} (2\pi)^{-1} \int_{-\infty}^{\infty} e^{i\,Et}\, dt . \tag{5.29}$$

This leads to the purely formal equation

$$\delta(E' - E') \longrightarrow (2\pi)^{-1} \int_{-\infty}^{\infty} dt \tag{5.30}$$

which we shall have occasion to comment on later.

6. LEVEL SHIFTS

Construction of the eigenvectors of H.

The operators $\bar{U}(0,\mp\infty)$ have now been given a clear definition, and we may proceed to write Eq. (4.30) in the form

$$|\zeta_\pm'\rangle = \bar{U}(0,\mp\infty)|\zeta_0'\rangle = \frac{\pm i\epsilon}{E' - H \pm i\epsilon}|\zeta_0'\rangle , \tag{6.1}$$

which follows from (5.21) and (2.13). Here, in addition to the vectors $|\zeta_+'\rangle$ representing retarded-wave solutions of the scattering problem, we have also introduced the advanced-wave solutions $|\zeta_-'\rangle$. Multiplication of Eq. (6.1) by $E' - H \pm i\epsilon$ yields $(E' - H)|\zeta_\pm'\rangle = 0$ in the limit $\epsilon \to 0$, showing that the $|\zeta_\pm'\rangle$ are indeed eigenvectors of H.

This construction of eigenvectors of H evidently works only if E' is an eigenvalue of H as well as of H_0, i.e. if there is no level shift. This condition is of course satisfied for the free states in simple scattering problems (Eq. (4.25)), but it is not generally satisfied for bound states, nor even for the free states of some complex systems, e.g. interacting fields. For bound states the construction (6.1) gives a vanishing result in the limit $\epsilon \to 0$ since E' is then generally not included in the spectrum of H and the denominator $E' - H \pm i\epsilon$ remains finite. Thus

$$\bar{U}(0,\mp\infty)|J_0'\rangle = 0 . \tag{6.2}$$

Construction (6.1) may, however, be salvaged for general use through a simple reselection of the unperturbed Hamiltonian operator. Let the level shift (if any) of the state $|\alpha_0'\rangle$ be denoted by $\Delta E'$ so that

$$H' = H_0' + \Delta E' . \tag{6.3}$$

The $\Delta E'$ are of course unknown in advance and must be computed in the course of solution of the problem. In sections 9 and 10 it will be shown how these level shifts may be determined, but for the present this question will be set aside. Introduce the operators

$$\Delta H_0 = \sum{}' |\alpha_0'\rangle \Delta E' \langle\alpha_0'| , \tag{6.4}$$

$$\mathcal{H}_0 = H_0 + \Delta H_0 , \tag{6.5}$$

$$\mathcal{H}_1 = H_1 - \Delta H_0 . \tag{6.6}$$

ΔH_0 commutes with H_0, and the $|\alpha_0'\rangle$ are eigenvectors of $\mathcal{H}_0$ as well as of H_0. If $\mathcal{H}_0$ is taken instead of H_0 as the unperturbed Hamiltonian, and if $\mathcal{H}_1$ is regarded as the perturbation, then no level shift occurs, and

$$E' = \mathcal{H}_0' = H' . \tag{6.7}$$

Construction (6.1) may therefore be used for <u>all</u> eigenstates of H which have counterparts in H_0 if one writes

$$Z'^{\frac{1}{2}} |\alpha_\pm'\rangle = \bar{\mathcal{U}}(0, \mp\infty)|\alpha_0'\rangle = \frac{\pm i\epsilon}{E' - H \pm i\epsilon} |\alpha_0'\rangle \tag{6.8}$$

where $\bar{\mathcal{U}}(t'', t')$ is the modified transformation operator in the interaction representation defined by the new operators $\mathcal{H}_0, \mathcal{H}_1$, and $Z'^{\frac{1}{2}}$ is a positive real normalizing factor, the necessity for which will presently become apparent. It is to be remembered that E' in (6.8) is now an eigenvalue of the total Hamiltonian operator H.

The normalization constant.

The normalization constant Z' has a simple physical significance which may easily be seen by multiplying the vector $|\alpha_\pm'\rangle$ by the Hermitian adjoint of Eq. (6.8) and observing that

$$\frac{\mp i\epsilon}{E' - H \mp i\epsilon}\,|\alpha_\pm'\rangle = |\alpha_\pm'\rangle \tag{6.9}$$

in the limit $\epsilon \to 0$. This relation together with the requirement $\langle\alpha_\pm'|\alpha_\pm'\rangle = 1$ leads to

$$Z'^{\frac{1}{2}} = \langle\alpha_0'|\alpha_\pm'\rangle \quad . \tag{6.10}$$

Z' is the probability of finding the unperturbed state $|\alpha_0'\rangle$ in the perturbed state $|\alpha_\pm'\rangle$.* Therefore

$$0 \leq Z' \leq 1 \, . \tag{6.11}$$

In the next section we shall see that $Z' = 1$ for the free states in simple scattering problems, so that Eq. (6.1) is still valid as it stands. Z' is generally different from unity, however, for problems involving bound states or interacting fields.

The case of bound states.

In the case of bound states there is a high degree of arbitrariness in the construction (6.8). It is apparent that $\pm i\epsilon(E' - H)/(E' - H \pm i\epsilon) \to 0$, so that the expression $\pm i\epsilon(E' - H \pm i\epsilon)^{-1}|\psi\rangle$ is, in the limit, an eigenvector of H corresponding to the eigenvalue E' regardless of the choice

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* That Z' is independent of the $\pm$ signs may be inferred by taking the scalar product of (6.8) with itself.

of the vector $|\psi\rangle$. Therefore the bound states of the two systems H_o and H can be paired off in any manner desired, the level shifts $\Delta E'$ being adjusted accordingly.

This arbitrariness does not exist in simple scattering problems nor in quantized field problems. For these problems there is a "natural" pairing of states between H_o and H which is determined first of all by a "natural" choice of H_o and, secondly, by the physically motivated procedure of adiabatic switching. We have seen that the validity of adiabatic switching for these problems depends on wave packet arguments. No such arguments exist in the case of bound states. However, there exists a celebrated theorem, which will be proved in section 9, which permits the extension of the adiabatic pairing process to bound systems as well as to all others. This <u>adiabatic theorem</u> states that a bound-state eigenvector of H_o is <u>dynamically</u> transformed into a bound-state eigenvector of H when the perturbation is switched on gradually, provided the vector is subject to certain well known restrictions (see end of this section) if H_o possesses degeneracy which is removed by the perturbation.

In the limit of vanishing ϵ, therefore, $|\alpha_\pm'\rangle$ may for bound states as well as free (with appropriate restrictions when degeneracy is removed) be defined as $\bar{U}^{ad}(0,\mp\infty)|\alpha_o'\rangle$ apart from a phase factor. Unfortunately, as we shall presently see, when a nonvanishing level shift occurs the phase factor oscillates infinitely fast as ϵ goes to zero. This prevents $\bar{U}^{ad}(0,\mp\infty)$ from being well defined in the limit. However,

the difficulty can be avoided by writing [34]

$$Z'^{-\frac{1}{2}} |\alpha_\pm'\rangle = \lim_{\epsilon \to 0} \frac{\bar{U}^{ad}(0, \mp\infty) |\alpha_0'\rangle}{\langle \alpha_0' | \bar{U}^{ad}(0, \mp\infty) | \alpha_0' \rangle} . \tag{6.12}$$

The numerator and denominator of this expression have the same oscillating phase, so the ratio is well defined. It is evident that the normalizing factor has been correctly chosen.*

Remaining arbitrariness.

Actually, the construction (6.12) still does not remove all the arbitrariness in the pairing of bound states. The pairing still depends on the operator H_0, and an eigenstate of H_0 which passes over into a certain eigenstate of H can be made to pass over into quite a different eigenstate of H if H_0 is redefined. This may be illustrated by the simple system

$$H = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \tag{6.13}$$

which has a discrete spectrum of only two levels, 0 and 2. A choice of H_0 according to

$$H_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad H_1 = \begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix}, \tag{6.14}$$

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* Evidently also, $\bar{\mathcal{U}}(0, \mp\infty) = \lim_{\epsilon \to 0} \bar{U}^{ad}(0, \mp\infty) \left[\bar{U}^{ad}(\mp\infty, 0) \right]_d$,

where $\left[\bar{U}^{ad}(\mp\infty, 0) \right]_d$ denotes the diagonal part of $\bar{U}^{ad}(\mp\infty, 0)$. (For definition section 11.)

leads to the adiabatic paring*

$$\begin{pmatrix}1\\0\end{pmatrix} \rightarrow \begin{pmatrix}1/\sqrt{2}\\1/\sqrt{2}\end{pmatrix}, \qquad \begin{pmatrix}0\\1\end{pmatrix} \rightarrow \begin{pmatrix}1/\sqrt{2}\\-1/\sqrt{2}\end{pmatrix}, \tag{6.15}$$

while the choice

$$H_o = \begin{pmatrix}-1 & 0\\0 & 1\end{pmatrix}, \qquad H_1 = \begin{pmatrix}2 & 1\\1 & 0\end{pmatrix}, \tag{6.16}$$

leads to the opposite pairing. The two choices correspond respectively to

$$\mathcal{H}_o = \begin{pmatrix}2 & 0\\0 & 0\end{pmatrix} \quad \text{and} \quad \mathcal{H}_o = \begin{pmatrix}0 & 0\\0 & 2\end{pmatrix}. \tag{6.17}$$

It is not possible to tamper with H_o in this manner in simple scattering and quantized field problems. In the simple scattering case it is possible to prove that $Z' = 1$ only if H_o is chosen in the usual manner, in which the remaining perturbation H_1 describes a force which is confined to a limited region of space. This last point is essential, as will be seen in the next section, and the proof would no longer hold if H_1 were redefined as in (6.6), since the arbitrary level shifts $\Delta E'$ would not correspond to a confined force. In fact, everything would break down, as one would consistently get $Z' \rightarrow 0$.

Contrastingly, in the case of quantized fields a redefinition of the type (6.4, 5, 6) is carried out precisely in order to cancel that part

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* Here it is sufficient to multiply H_1 in (6.14) by a variable χ, then to regard H as a function of χ and observe the continuous change of its eigenvectors as χ passes from 0 to 1.

of the interaction between field quanta which is unconfined (i.e., which exists no matter where a given quantum is located), the so called <u>self-interactions.</u> However, H_o must be chosen in a definite way, and there is no arbitrariness in the level shifts. (See section 10.)

In practice, of course, there is usually a "natural" choice for H_o even in bound state problems. Therefore the remarks about arbitrariness are largely academic, and we shall continue to assume that the correspondence between the eigenstates of the actual system H and those of the reference system is unique and well defined in all cases.

<u>Oscillating factors.</u>

The effect of the level shifts on the time behavior of the unmodified transformation operator $\bar{U}(t'', t')$ may be readily seen. From Eq. (2.20) and the commutativity of ΔH_o with H_o, one gets

$$\bar{U}(t'', t') = e^{-i \Delta H_o t''} \bar{\mathfrak{U}}(t'', t') e^{i \Delta H_o t'} , \tag{6.18}$$

or, in matrix form,

$$\langle \alpha_o'' | \bar{U}(t'', t') | \alpha_o' \rangle = e^{-i \Delta E'' t'' + i \Delta E' t'} \langle \alpha_o'' | \bar{\mathfrak{U}}(t'', t') | \alpha_o' \rangle . \tag{6.19}$$

When $\Delta E'$ or $\Delta E''$ is different from zero the corresponding matrix elements of $\bar{U}(t'', t')$ have oscillating factors. Because of these factors the matrix elements are forced, by the limiting convention (5.22), to vanish for $t', t'' = \pm\infty$, and results like (6.2) follow.

The fact that Z' is generally less than unity implies that $\bar{\mathfrak{U}}(t'', t')$ itself possesses additional oscillating parts which are eliminated by (5.22). Otherwise the unitarity of $\bar{\mathfrak{U}}(t'', t')$ would

guarantee the normalization of the vectors $|\alpha_\pm'\rangle$ without the factor $Z'^{\frac{1}{2}}$. The simple example (6.13) readily shows these extra oscillations. Using the first choice in (6.17) for $\mathcal{H}_0$, one has

$$\bar{\mathcal{U}}(0, t) = e^{iHt} e^{-i\mathcal{H}_0 t} = \frac{1}{2}\begin{pmatrix} 1 + e^{-2it} & e^{2it} - 1 \\ 1 - e^{-2it} & e^{2it} + 1 \end{pmatrix}, \tag{6.20}$$

yielding the non-unitary result

$$\bar{\mathcal{U}}(0, \mp\infty) = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \tag{6.21}$$

which leads to $Z' = \frac{1}{2}$ for both eigenstates of $\mathcal{H}_0$. The oscillations of $\bar{\mathcal{U}}(t'', t')$ generally do not occur multiplicatively.

The fact that the level shift oscillations in $\bar{U}(t'', t')$ do occur multiplicatively, allows one to determine the form in which the oscillating phase appears in $\bar{U}^{ad}(0, \mp\infty)$. Regard the adiabatic switching (5.1) as due to a time variation in the coupling constant of the form

$$dg/dt = \pm \epsilon g . \tag{6.22}$$

The level shifts $\Delta E'$ at any instant of time will be functions of g. The operators $\bar{U}^{ad}(0, \mp\infty)$ may be expressed as infinite products of factors $\bar{U}^{ad}(t, t + dt)$, each factor contributing an amount $\Delta E'(g)dt$ to the level shift phase for the state $|\alpha_0'\rangle$. The total phase change between 0 and $\mp\infty$ is evidently

$$\int_0^{\mp\infty} \Delta E'(g)dt = \mp \epsilon^{-1} \int_0^g \Delta E'(g) g^{-1}\, dg . \tag{6.23}$$

The matrix element $\langle \alpha_o' | \bar{U}^{ad}(0, \mp\infty) | \alpha_o' \rangle$ will therefore have as a factor $\exp\left[(\pm i\epsilon)^{-1} \int_0^g \Delta E'(g) g^{-1}\, dg \right]$. Its other factors will depend on ϵ in a much less singular way. Hence one may write

$$\Delta E' = \lim_{\epsilon \to 0} \pm i\epsilon g\, \partial \ln \langle \alpha_o' | \bar{U}^{ad}(0, \mp\infty) | \alpha_o' \rangle / \partial g \quad (6.24)$$

<u>Rigorous derivation of Eq. (6.24).</u>

Eq. (6.24) is useful theoretically although it is not to be regarded as providing a practical method for the calculation of level shifts. It may be derived in a more rigorous fashion by using the time-ordered expansions (1.31b) and (1.32b) of the interaction transformation operator, and the equation of motion (1.26) for operators in the interaction representation. One writes [34]

$$(H_o' - H_o)\bar{U}^{ad}(0, \mp\infty) | \alpha_o' \rangle = \left[\bar{U}^{ad}(0, \mp\infty), H_o \right] | \alpha_o' \rangle$$

$$= \left[\left[\exp\left(i \int_0^{\mp\infty} \bar{H}_1^{ad}(t)dt\right) \right]_\pm , H_o \right] | \alpha_o' \rangle$$

$$= \sum_{n=1}^{\infty} (i^{n+1}/n!) \int_0^{\mp\infty} dt_1 \ldots \int_0^{\mp\infty} dt_n\, e^{\pm\epsilon(t_1 + \ldots + t_n)}$$

$$\sum_{m=1}^{n} \partial \left[\bar{H}_1(t_1) \ldots \bar{H}_1(t_n) \right]_\pm / \partial t_m | \alpha_o' \rangle$$

$$= - \sum_{n=1}^{\infty} \left[i^{n-1}/(n-1)! \right] \int_0^{\mp\infty} dt_1 \ldots \int_0^{\mp\infty} dt_n\, e^{\pm\epsilon(t_1 + \ldots + t_n)}$$

$$\partial \left[\bar{H}_1(t_1) \ldots \bar{H}_1(t_n) \right]_\pm / \partial t_n | \alpha_o' \rangle$$

$$= (H_1 \mp i\epsilon g \partial / \partial g) \bar{U}^{ad}(0, \mp\infty) | \alpha_o' \rangle \quad . \quad (6.25)$$

Advantageous use of the time-ordering brackets is made here. The final form is obtained by a partial integration and the observation that the result is equivalent to an application of the operator $H_1 \mp i\epsilon g \partial/\partial g$ in the manner indicated. The operator $H_1 = \bar{H}_1(0)$ comes from an evaluation at the lower limit of integration, the time-ordering brackets insuring that it stands to the left. Eq. (6.25) may also be derived by working directly with the expansion (5.5). [41]

Using (6.12) and (6.25), and letting the limit $\epsilon \to 0$ be understood one may now write

$$0 \leftarrow \mp i\epsilon g \partial |\alpha_\pm'\rangle / \partial g$$

$$= \mp i\epsilon Z'^{\frac{1}{2}} g \left[\frac{\partial \bar{U}^{ad}(0,\mp\infty)|\alpha_0'\rangle / \partial g}{\langle\alpha_0'|\bar{U}^{ad}(0,\mp\infty)|\alpha_0'\rangle} - \frac{\partial \langle\alpha_0'|\bar{U}^{ad}(0,\mp\infty)|\alpha_0'\rangle / \partial g}{\langle\alpha_0'|\bar{U}^{ad}(0,\mp\infty)|\alpha_0'\rangle^2} \bar{U}^{ad}(0,\mp\infty)|\alpha_0'\rangle \right]$$

$$= \left[H_0' \pm i\epsilon g \partial \ln \langle\alpha_0'|\bar{U}^{ad}(0,\mp\infty)|\alpha_0'\rangle / \partial g - H \right] |\alpha_\pm'\rangle \quad , \tag{6.26}$$

which leads to the identification (6.24) for the level shifts. The vanishing limit expressed by the first line of (6.26) occurs because $|\alpha_\pm'\rangle$, unlike $\bar{U}^{ad}(0,\mp\infty)|\alpha_0'\rangle$, does not depend on ϵ in a singular way.

Eq. (6.24) may actually be generalized to

$$\langle\alpha_0''|\bar{U}^{ad}(0,\mp\infty)|\alpha_0'\rangle \Delta E' = \pm i\epsilon g \partial \langle\alpha_0''|\bar{U}^{ad}(0,\mp\infty)|\alpha_0'\rangle / \partial g \tag{6.27}$$

for arbitrary $\langle\alpha_0''|$ (the limit $\epsilon \to 0$ being understood) since the oscillating phase factor is independent of $\langle\alpha_0''|$. Multiplying (6.27) on the left by $\bar{U}^{ad}(\mp\infty, 0)|\alpha_0''\rangle$ and on the right by $\langle\alpha_0'|$, and summing over α_0' and α_0'', one gets

$$\Delta H_0 = \pm i\epsilon g \bar{U}^{ad}(\mp\infty, 0)\, \partial \bar{U}^{ad}(0, \mp\infty)/\partial g , \tag{6.28}$$

which, together with (6.25), gives the concise statement

$$H_0 + \Delta H_0 = \bar{U}^{ad}(\mp\infty, 0) H \bar{U}^{ad}(0, \mp\infty) . \tag{6.29}$$

Some remarks.

Several final remarks should be make. The first is that those eigenstates of H which have no counterparts in H_0 (if any) cannot be constructed by schemes based on (6.8) or (6.12). They must be found by independent and generally more difficult means. The second is that if any of the states $|\alpha_0'\rangle$ has no counterpart in H, because it undergoes decay for example, then the normalization constant Z' vanishes for that state and the symbol $|\alpha_\pm'\rangle$ is meaningless.*

The third remark is that the redefinition (6.4, 5, 6) is not the only possible one which eliminates the level shifts. In relativistic field theories ΔH_0 generally does not commute with H_0 but is chosen in such a way as to maintain the manifest covariance of a relativistic

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* In this case Z' is rigorously zero. In divergent field theories one sometimes encounters the equation $Z' = 0$, but what is meant is only that Z' becomes vanishingly small as the high energy cut-off is allowed to become infinite. As long as the cut-off remains finite Z' is finite and the state vector $|\alpha_\pm'\rangle$ can be normalized. The symbol $|\alpha_\pm'\rangle$ then retains meaning even in the limit.

formalism. However, the choice (6.4) is sufficiently typical and illustrates all the features of the process. In fact it differs from the relativistic choice only in that it may be described as a renormalization of energy, which is not a relativistic invariant, while the relativistic choice is a renormalization of rest mass, which is invariant. The one is generally only a slight modification of the other.

The last remark concerns degeneracy. If there is degeneracy which is removed, at least in part, by the switching on of the perturbation then the construction (6.12) will work only if the vectors $|\alpha_0'\rangle$ are suitably chosen, viz: they must be the limiting forms of the eigenvectors of H as the perturbation is switched off. This requirement evidently leads to a vicious circle as far as practical applications are concerned, since the eigenvectors of H are generally not known in advance. Therefore, in the presence of degeneracy, Eq. (6.12) must be understood as having theoretical utility only.

The situation arises mainly in bound state perturbation theory,* and there one has several methods of dealing with it practically. Two of these methods will be outlined in section 9, one which deals directly with the projection operators arising from the degenerate levels, and the other which systematically redefines H_0 so that all the removable degeneracy is removed in advance.

It will also be seen in section 9 that it does not matter whether the bound-state eigenvectors of the system H are obtained by adiabatic switching from the remote past or the remote future; the result will be the same in either case. That is to say, $|\alpha_+'\rangle = |\alpha_-'\rangle$, and the symbols $\pm$ become superfluous. This is true even in the presence of unremoved degeneracy, for which construction (6.12) is valid without restriction. It is not, however, generally true for free states, for which unremoved degeneracy is the rule rather than the exception. Thus, in scattering problems, the $\pm$ signs are not superfluous. In passing all the way from $-\infty$ to $+\infty$, the perturbation being switched on and then off again, the $|\alpha_0'\rangle$ will become shuffled around, winding up in new iso-energetic combinations.

* The situation may also arise in field theories for which the coupling is asymmetric (see section 10). The proper choice of unperturbed vectors is then usually obvious, however.

7. SCATTERING CONTINUED

The orthonormality of the vectors $|\zeta_\pm'\rangle$.

The first task of this section will be to prove the orthonormality of the free-state vectors $|\zeta_\pm'\rangle$ as defined by (6.1). For this and many other subsequent purposes it will be convenient to introduce the following auxilliary operators:*

$$R_\pm = H_1 \bar{U}(0, \mp\infty)$$

$$= \sum{}' R_\pm(E')|\alpha_0'\rangle\langle\alpha_0'| \quad , \tag{7.1}$$

where

$$R_\pm(E') = H_1 \left[1 - G_{0\pm}(E')\, H_1\right]^{-1} \tag{7.2a}$$

$$= \left[1 - H_1\, G_{0\pm}(E')\right]^{-1} H_1 \tag{7.2b}$$

$$= H_1 + H_1\, G_\pm(E')\, H_1 \tag{7.3}$$

$$= H_1 \left[1 + G_{0\pm}(E')\, R_\pm(E')\right] \tag{7.4a}$$

$$= \left[1 + R_\pm(E')\, G_{0\pm}(E')\right] H_1 \quad . \tag{7.4b}$$

Eq. (7.2a) follows from (5.20). The remaining forms may be obtained either by expanding and comparing terms or by using Eqs. (2.14) and (2.16) judiciously. By similar algebraic manipulation one may also write Eq. (6.1) in the forms

$$|\zeta_\pm'\rangle = \left[1 - G_{0\pm}(E')\, H_1\right]^{-1} |\zeta_0'\rangle \tag{7.5}$$

$$= \left[1 + G_\pm(E')\, H_1\right] |\zeta_0'\rangle \tag{7.6}$$

$$= |\zeta_0'\rangle + G_{0\pm}(E')\, H_1 |\zeta_\pm'\rangle \tag{7.7}$$

$$= \left[1 + G_{0\pm}(E')\, R_\pm(E')\right] |\zeta_0'\rangle \quad . \tag{7.8}$$

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* The operator $R_\pm$ is often denoted in the literature by $T^{(\pm)}$. Frequent use is also made of a symbol $\Omega^{(\pm)}(E) \equiv \left[1 - G_{0\pm}(E) H_1\right]^{-1}$ such that $\bar{U}(0, \mp\infty) = \sum{}' \Omega^{(\pm)}(E')|\alpha_0'\rangle\langle\alpha_0'|$.

The proof of the orthonormality of the $|\zeta_\pm'\rangle$ depends on careful handling of limits. One must not allow ϵ to vanish too soon. Thus, from (6.1),

$$(E' - H)|\zeta_\pm'\rangle = \pm i\epsilon(|\zeta_0'\rangle - |\zeta_\pm'\rangle) . \tag{7.9}$$

This equation and its conjugate yield the identity

$$\begin{aligned} 0 &= \langle\zeta_\pm''|(E' - H)|\zeta_\pm'\rangle - \langle\zeta_\pm''|[(E'' - H) + (E' - E'')]|\zeta_\pm'\rangle \\ &= -(E' - E'' \pm 2i\epsilon)\langle\zeta_\pm''|\zeta_\pm'\rangle \pm i\epsilon\left(\langle\zeta_\pm''|\zeta_0'\rangle + \langle\zeta_0''|\zeta_\pm'\rangle\right), \end{aligned} \tag{7.10}$$

which in turn, with the aid of (7.8), gives

$$\begin{aligned} \langle\zeta_\pm''|\zeta_\pm'\rangle &= \frac{\pm i\epsilon}{E' - E'' \pm 2i\epsilon}\Big[2\delta(\zeta_0'',\zeta_0') + \langle\zeta_0''|R_\mp(E'')G_{0\mp}(E'')|\zeta_0'\rangle \\ &\qquad + \langle\zeta_0''|G_{0\pm}(E')\,R_\pm(E')|\zeta_0'\rangle\Big] \\ &= \delta(\zeta_0'',\zeta_0') \mp \frac{2\epsilon}{(E' - E'' \pm 2i\epsilon)(E' - E'' \pm i\epsilon)}\langle\zeta_0''|\operatorname{Im} R_\pm|\zeta_0'\rangle \\ &\rightarrow \begin{cases} 0 , & E'' \neq E' \\ \delta(\zeta_0'',\zeta_0') \pm \epsilon^{-1}\langle\zeta_0''|\operatorname{Im} R_\pm|\zeta_0'\rangle , & E'' = E' , \end{cases} \end{aligned} \tag{7.11}$$

where the obvious relations

$$G_{0\pm}(E')^* = G_{0\mp}(E') , \qquad R_\pm(E')^* = R_\mp(E') , \tag{7.12}$$

have been used, and $\operatorname{Im} R_\pm$ is $-i$ times the skew-Hermitian (imaginary) part of $R_\pm$. The orthonormality of the $|\zeta_\pm'\rangle$ will follow from (7.11) if

$$\lim_{\epsilon \to 0} \epsilon^{-1} \left\langle \zeta_0'' \middle| \mathrm{Im}\, R_\pm \middle| \zeta_0' \right\rangle = 0 . \tag{7.13}$$

Proof of Eq. (7.13) in the case of simple scattering.

It will now be shown that (7.13) is a correct equation for simple scattering problems, but only as the result of a certain necessary double limiting process.

In order that the normalization condition (1.35) be imposable on the free-state basic vectors $|\zeta_0'\rangle$ it is necessary that the system be placed in a box, which is conveniently taken as rectangular with side L. If the coordinates q' of the system are introduced,* the free-state eigenfunctions $\langle q' | \zeta_0' \rangle$ will be proportional to $(L^{-N}\, d^N q')^{\frac{1}{2}}$ where $d^N q'$ is the volume element in coordinate space and N is the number of degrees of freedom. Consider the matrix element

$$\left\langle \zeta_0'' \middle| H_1 \middle| \zeta_0' \right\rangle = \sum_{q',q''} \left\langle \zeta_0'' \middle| q'' \right\rangle \left\langle q'' \middle| H_1 \middle| q' \right\rangle \left\langle q' \middle| \zeta_0' \right\rangle \tag{7.14}$$

of the perturbation operator H_1. Its coordinate matrix elements $\left\langle q'' \middle| H_1 \middle| q' \right\rangle$ are proportional to $(d^N q''\, d^N q')^{\frac{1}{2}}$ so that the right-hand side of (7.14) becomes a double integral. Now, one of the requirements on the scattering force is that it be confined to a limited region of space (see section 4). This means that the matrix element $\left\langle q'' \middle| H_1 \middle| q' \right\rangle$ must vanish when q' or q'' is outside of this region. The integration in (7.14) is therefore convergent,** and the result is of order L^{-N}.

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* The inclusion of spin or other variables is irrelevant for the present argument.

** This also assumes the forces are not too singular at the origin.

We write

$$\langle \zeta_0'' | H_1 | \zeta_0' \rangle = O(L^{-N}) . \tag{7.15}$$

By similar reasoning it is evident that the corresponding matrix element of each term of the expansion of (7.2a) is of order L^{-N}, and hence that*

$$\langle \zeta_0'' | R_\pm | \zeta_0' \rangle = O(L^{-N}), \tag{7.16}$$

the expansion being evaluated by analytic continuation if necessary. Eq. (7.16) must hold separately for both the real and imaginary parts of $R_\pm$, and therefore

$$\epsilon^{-1} \langle \zeta_0'' | \mathrm{Im}\, R_\pm | \zeta_0' \rangle = O(\epsilon^{-1} L^{-N}). \tag{7.17}$$

Eq. (7.13) can follow from (7.17) only if, as ϵ vanishes, L becomes infinite rapidly enough to make $\epsilon^{-1} L^{-N}$ infinitesimal. The necessity for this, however, can be shown by two arguments. The first is a physical argument and is based on the wave packet picture: If v is the group velocity of a packet then L/v is the length of time it takes for the packet to traverse the enclosing box. This time must always be much greater than the time $2/\epsilon$ of duration of the perturbation, if the

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* Eqs. (7.15) and (7.16) are actually satisfied by a much wider class of potentials than those which are strictly confined to a limited region of space. The confinement restriction can be replaced by weaker conditions concerning the rapidity with which the potential vanishes at large distance Eq. (7.15) by itself, however, is not sufficient to express these conditions, as is shown by the well known example of the Coulomb potential, for which (7.15) holds although $\langle \zeta_0'' | R | \zeta_0' \rangle$ is divergent. There is strong evidence that the Coulomb case can nevertheless be analyzed by the formalistic techniques of the present article in terms not only of the well known infinite phase shift but also of a <u>simultaneous state vector renormalization</u>, although such an analysis has never been carried out, to the author's knowledge.

adiabatic switching procedure is to provide an adequate mathematical substitute for the actual scattering process in which the packet moves unperturbed both before and after scattering. Therefore

$$\epsilon^{-1} L^{-1} \rightarrow 0 \ . \tag{7.18}$$

which leads to (7.13) for all N.

The seconr argument is more mathematical: When the system is placed in the box the energy levels necessarily become discrete, the level spacing being of order L^{-1}. In order that the imaginary parts $\pm i\epsilon$ of the "energy denominators" of the Green's functions $G_{0\pm}(E)$ give the correct causal description of the scattering process (i.e., be able to distinguish between retarded and advanced wave solutions), ϵ must be much larger than the level spacing so that the summation over intermediate states will take on a <u>fine-grained</u> aspect with respect to ϵ and be representable as an integral over a contour which passes definitely to one side or the other of the energy pole. This argument again gives (7.18), and the orthonormality of the $|\zeta_\pm'\rangle$ is therefore proved.

<u>The case $Z' < 1$.</u>

In those cases in which the normalization constant Z' of Eq. (6.8) is different from unity, Eq. (7.11) may be used to determine its value. Here we work with the operators

$$\mathcal{R}_\pm = \mathcal{H}_1 \bar{\mathcal{U}}(0, \mp\infty) \tag{7.19}$$

$$= \text{Sing}\, \mathcal{R}_\pm + R_\pm \ . \tag{7.20}$$

The notation "Sing" separates out that part of $\mathcal{R}_\pm$ which has matrix elements independent of L, i.e. the "singular" part of $\mathcal{R}_\pm$. For bound states $\mathcal{R}_\pm$ has no nonsingular part $R_\pm$. For the free states in

quantized field theories the matrix elements of $R_\pm$ are of order L^{-N}, the exponent N depending on the number of field quanta involved. Therefore, while $R_\pm$ is all important as far as scattering is concerned, it does not affect the normalization and may be neglected in the present discussion.

For orthonormality of the vectors $|\alpha_\pm{}'\rangle$ one must first be able to show that

$$\langle\alpha_0{}''|\,\mathrm{Im\ Sing}\,\mathcal{R}_\pm\,|\alpha_0{}'\rangle = \mp\epsilon\Lambda'\delta(\alpha_0{}'',\alpha_0{}'), \quad E'' = E' , \tag{7.21}$$

where the Λ' are positive real numbers independent of ϵ and L, and then one must choose

$$Z' = 1 - \Lambda' . \tag{7.22}$$

In bound state problems Eq. (7.21) follows as a consequence of those symmetries of the perturbation which leave degeneracies in the system. In sec. 10 it will also be seen to hold in quantized field theories.

The symbol Im in (7.21) is actually unnecessary. It will be seen in section 9 that in the case of bound states, if there is any unremoved degeneracy,

$$\langle\alpha_0{}''|\alpha_\pm{}'\rangle = Z'^{\frac{1}{2}}\delta(\alpha_0{}'',\alpha_0{}'), \qquad E'' = E' . \tag{7.23}$$

This, combined with the obvious generalization of Eq. (7.8), gives

$$Z'\delta(\alpha_0{}'',\alpha_0{}') = \delta(\alpha_0{}'',\alpha_0{}') + (\pm i\epsilon)^{-1}\langle\alpha_0{}''|\mathrm{Sing}\,\mathcal{R}_\pm|\alpha_0{}'\rangle \qquad , E'' = E' , \tag{7.24}$$

or

$$\langle\alpha_0{}''|\mathrm{Sing}\,\mathcal{R}_\pm|\alpha_0{}'\rangle = \mp i\epsilon\Lambda'\delta(\alpha_0{}'',\alpha_0{}'), \qquad E'' = E' . \tag{7.25}$$

This result will also hold in the case of quantized fields.

Use of these equations may be readily illustrated with the simple system (6.13). One gets, with the first choice in (6.17),

$$\mathcal{R}_{\pm}|\alpha_0'\rangle = \mathcal{H}_1 \frac{\pm i\epsilon}{E' - H \pm i\epsilon}|\alpha_0'\rangle$$

$$= \begin{cases} \dfrac{\pm i\epsilon}{\pm 2i\epsilon - \epsilon^2} \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \pm i\epsilon & 1 \\ 1 & 1 \pm i\epsilon \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow \frac{1}{2}\begin{pmatrix} \pm i\epsilon \\ 2 \end{pmatrix}, & E' = 2 \\[2ex] \dfrac{\pm i\epsilon}{\mp 2i\epsilon - \epsilon^2} \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} -1 \pm i\epsilon & 1 \\ 1 & -1 \pm i\epsilon \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow \frac{1}{2}\begin{pmatrix} 2 \\ \mp i\epsilon \end{pmatrix}, & E' = 0 \end{cases}$$

yielding the previously inferred result $\Lambda' = \frac{1}{2}$, $Z' = \frac{1}{2}$ for both states.

The illustration with quantized fields will be given in section 10.

<u>Orthogonality of $|\mathfrak{J}_{\pm}'\rangle$ and $|J'\rangle$.</u>

Returning now to simple-scattering problems, we note that since the $|\mathfrak{J}_{\pm}'\rangle$ are free-state vectors of the system H, they are orthogonal to any bound-state eigenvectors $|J'\rangle$ which H may have:

$$\langle \mathfrak{J}_{\pm}''|J'\rangle = 0 . \tag{7.26}$$

This follows immediately from Eq. (6.1) multiplied by $\langle J'|$. It also follows indirectly from the observation that the expression $e^{iH_0t}\, e^{-iHt}$ may be interpreted not only (by (2.20)) as the transformation operator $\bar{U}(t, 0)$ from time 0 to time t in the interaction representation of system H, with H_0 as the reference system, but also as the transformation operator from time t to time 0 in the interaction representation of system H_0, with H as the reference system. Therefore by reasoning

identical with that leading to Eq. (6.2) one gets

$$\bar{U}(\mp\infty, 0)\,|J'\rangle = \frac{\pm i\epsilon}{H' - H_0 \pm i\epsilon}\,|J'\rangle \longrightarrow 0 \;, \tag{7.27}$$

the roles of the two systems now being inverted. Expression (7.27) vanishes in the limit since H' is not generally included* in the spectrum of H_0. This equation can be obtained directly through use of the limiting convention (5.22). Multiplication on the left by $\langle \mathfrak{J}_0''|$ gives (7.26).

Question of unitarity.

It is now possible to discuss the unitarity of the operators $\bar{U}(0,\mp\infty)$ and $\bar{U}(\pm\infty,\mp\infty)$. Eqs. (6.1), (6.2) and (7.27) evidently allow one to write

$$\bar{U}(0,\mp\infty) = \sum{}' \,|\mathfrak{J}_\pm'\rangle\langle\mathfrak{J}_0'| \,. \tag{7.28}$$

Therefore, owing to the orthonormality of the $|\mathfrak{J}_\pm'\rangle$ and of the $|\mathfrak{J}_0'\rangle$,

$$\bar{U}(0,\mp\infty)^*\,\bar{U}(0,\mp\infty) = \sum{}' \,|\mathfrak{J}_0'\rangle\langle\mathfrak{J}_0'| = P_{\mathfrak{J}_0} \tag{7.29a}$$

$$= 1 - P_{J_0} \;, \tag{7.29b}$$

$$\bar{U}(0,\mp\infty)\,\bar{U}(0,\mp\infty)^* = \sum{}' \,|\mathfrak{J}_\pm'\rangle\langle\mathfrak{J}_\pm'| = P_{\mathfrak{J}} \tag{7.30a}$$

$$= 1 - P_J \;. \tag{7.30b}$$

where $P_{\mathfrak{J}_0}$ and $P_{\mathfrak{J}}$ are the free-state projection operators for the systems H_0 and H respectively, and P_{J_0} and P_J are the bound-state projection operators.

$$P_{J_0} = \sum{}' \,|J_0'\rangle\langle J_0'| \;, \qquad P_J = \sum{}' \,|J'\rangle\langle J'| \;. \tag{7.31}$$

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* For simplicity in this discussion of bound states we exclude cases in which some of the bound levels of H and H_0 coincide.

The equations $P_{\mathcal{J}_0} + P_{J_0} = P_{\mathcal{J}} + P_J = 1$ express the completeness condition for the eigenvectors of the two systems. It is seen that if either of the systems has bound states the operators $\bar{U}(0, \mp\infty)$ are not strictly unitary.

From Eqs. (5.8), (5.24), (5.25), (7.27), (7.29), (7.30), one gets [30]

$$\bar{U}(\pm\infty, \mp\infty)^* \bar{U}(\pm\infty, \mp\infty)$$

$$= \bar{U}(\mp\infty, 0)\, \bar{U}(0, \pm\infty)\, \bar{U}(\pm\infty, 0)\, \bar{U}(0, \mp\infty)$$

$$= \bar{U}(\mp\infty, 0)(1 - P_J)\, \bar{U}(0, \mp\infty) = P_{\mathcal{J}_0} \quad , \tag{7.32}$$

or

$$S^* S = S S^* = P_{\mathcal{J}_0} \quad . \tag{7.33}$$

Therefore the unitarity of the scattering operator, unlike that of the operators $\bar{U}(0, \mp\infty)$, depends only on the comparison system H_0. If, as is so often the case in practice, H_0 has no bound states, then the scattering operator is strictly unitary regardless of whether or not the system H has bound states.

For systems involving quantized fields analagous quasi-unitary operators may be obtained by "renormalizing" the operators $\bar{\mathcal{U}}(0, \mp\infty)$. Denote by $|\gamma_0'\rangle$ the states of H_0 which undergo decay or otherwise have no counterparts in H. Denote the remaining states by $|\beta_0'\rangle$. Then the "renormalized" or "corrected" operators are defined by

$$\bar{\mathcal{U}}_c(0, \mp\infty) = \sum{}' |\beta_\pm'\rangle\langle\beta_0'| = \bar{\mathcal{U}}(0, \mp\infty) \sum{}' |\beta_0'\rangle Z'^{-\frac{1}{2}} \langle\beta_0'| \quad , \tag{7.34}$$

$$S_c = \bar{\mathcal{U}}_c(\infty, 0)\, \bar{\mathcal{U}}_c(0, -\infty) \quad . \tag{7.35}$$

Evidently

$$S_c^* S_c = S_c S_c^* = P_{\beta_0} = 1 - P_{\gamma_0} , \tag{7.36}$$

P_{β_0} and P_{γ_0} being the projection operators on the states $|\beta_0'\rangle$ and the states $|\gamma_0'\rangle$ respectively.

The scattering operator for other important complex systems will be defined in section 12.*

Structure of the S-matrix.

We shall now carry out an explicit construction of the scattering operator. For this purpose three simple identities will be needed. First, from Eqs. (2.16) and (7.2),

$$G_\pm(E')H_1 = G_{0\pm}(E')R_\pm(E') , \qquad H_1 G_\pm(E') = R_\pm(E') G_{0\pm}(E') . \tag{7.37}$$

Second, from Eqs. (2.13) and (7.3),

$$R_\pm(E'') - R_\pm(E') = (E' - E'')H_1 G_\pm(E'') G_\pm(E')H_1 . \tag{7.38}$$

The third identity results from taking the limit $E'' \rightarrow E'$ in (7.38):

$$\partial R(E')/\partial E' = - H_1 \left[G_\pm(E')\right]^2 H_1 . \tag{7.39}$$

Using these identities together with Eq. (7.8), one may write the elements of the S-matrix and its Hermitian adjoint in the form

$$\langle \zeta_0'' | \bar{U}(\pm\infty, \mp\infty) | \zeta_0' \rangle = \langle \zeta_\mp'' | \zeta_\pm' \rangle$$

$$= \langle \zeta_0'' | \left[1 + R_\pm(E'')G_{0\pm}(E'')\right]\left[1 + G_{0\pm}(E') R_\pm(E')\right] | \zeta_0' \rangle$$

$$= \delta(\zeta_0'', \zeta_0') + \frac{\frac{1}{2}}{E'' - E' \pm i\epsilon} \langle \zeta_0'' | \left[R_\pm(E'') + R_\pm(E') + (E' - E'')H_1 G_\pm(E'')G_\pm(E')H_1\right] | \zeta_0' \rangle$$

$$\frac{\frac{1}{2}}{E' - E'' \pm i\epsilon} \langle \zeta_0'' | \left[R_\pm(E'') + R_\pm(E') + (E'' - E')H_1 G_\pm(E'')G_\pm(E')H_1\right] | \zeta_0' \rangle$$

$$+ \langle \zeta_0'' | H_1 G_\pm(E'') G_\pm(E') H_1 | \zeta_0' \rangle$$

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* For bound systems the scattering operator reduces to the triviality $S_c = 1$.

$$= \delta(\zeta_0'', \zeta_0') \mp \frac{i\epsilon}{(E'' - E')^2 + \epsilon^2} \left\langle \zeta_0'' \right| \left[R_\pm(E'') + R_\pm(E') \right] \left| \zeta_0' \right\rangle$$

$$+ \frac{\epsilon^2}{(E'' - E')^2 + \epsilon^2} \left\langle \zeta_0'' \right| H_1 \, G_\pm(E'') \, G_\pm(E') \, H_1 \left| \zeta_0' \right\rangle$$

$$\longrightarrow \delta(\zeta_0'', \zeta_0') \mp 2\pi i \, \delta(E'' - E') \left[\left\langle \zeta_0'' \right| R_\pm \left| \zeta_0' \right\rangle \mp \tfrac{1}{2} i\epsilon \left\langle \zeta_0'' \right| \partial R_\pm(E')/\partial E' \left| \zeta_0' \right\rangle \right] \tag{7.40}$$

The S-matrix is seen to have nonvanishing elements only for states with equal energies. This is a statement of the fact that the energy of the <u>unperturbed</u> system is conserved under a collision. It is useful to indicate here several other ways of obtaining the same result. First, since $H_0' = H' = E'$ for the states $|\zeta_0'\rangle$, $|\zeta_\pm'\rangle$, use of Eq. (7.28) enables one to write*

$$H \, \bar{U}(0, \mp\infty) = \bar{U}(0, \mp\infty) H_0 \, . \tag{7.41}$$

This equation together with its Hermitian adjoint and Eq. (5.8) yields

$$\left[S, H_0 \right] = 0 \, , \tag{7.42}$$

which is the operator statement of conservation of energy. Eq. (7.42) also follows from (1.26) and the special cases of Eqs. (1.31b), (1.32b), viz.,

$$\bar{U}(\pm\infty, \mp\infty) = \left[\exp\left(\mp i \int_{-\infty}^{\infty} \bar{H}_1(t) dt\right) \right]_\pm P_{\zeta_0} \, . \tag{7.43}$$

The displacement in time effected by taking the commutator with H_0 leaves

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* A related equation, namely $\zeta_\pm = \bar{U}(0, \mp\infty) \; \zeta_0 \; \bar{U}(\mp\infty, 0)$, gives an explicit definition to the operators $\zeta_\pm$ which, up to now, have been largely undetermined, their role having been confined merely to one of providing suitable labels for the eigenvectors of H.

S unchanged since the integrations in (7.43) run from $t = -\infty$ to $t = +\infty$. Finally, Eq. (7.41) may be combined with Eqs. (5.23) and (2.20) to yield once again Eq. (5.17), which, when combined with the integral equation (1.30a) and the integral representation of the delta function (Eq. (5.30)), gives

$$\begin{aligned}\bar{U}(\pm\infty, \mp\infty) &= \left[1 \mp i\int_{-\infty}^{\infty} \bar{H}_1(t)\, \bar{U}(t, \mp\infty)dt\right] P_{\zeta_0} \\ &= P_{\zeta_0} \mp i \sum{}' \int_{-\infty}^{\infty} e^{i(H_0 - E')t} H_1\, \bar{U}(0, \mp\infty)dt\, |\zeta_0'\rangle\langle\zeta_0'| \\ &= P_{\zeta_0} \mp i\, \underset{\sim}{R}_{\pm} \qquad (7.44)\end{aligned}$$

where

$$\underset{\sim}{R}_{\pm} = 2\pi \sum{}' \delta(E' - H_0)\, R_{\pm}\, |\zeta_0'\rangle\langle\zeta_0'| \qquad (7.45a)$$

$$= 2\pi \sum{}' |\zeta_0'\rangle\langle\zeta_0'|\, R_{\pm}\, \delta(E' - H_0) \qquad (7.45b)$$

satisfying

$$\underset{\sim}{R}_{\pm}^{*} = \underset{\sim}{R}_{\pm} \,. \qquad (7.46)$$

In Eqs. (7.43, 44) we have been careful to multiply by the projection operator P_{ζ_0}, since the removal of the oscillating components of the interaction transformation operator, which is implied by the limiting convention (5.22), is <u>not</u> implied by the integral equations (1.30).

Eq. (7.44) is the operator form of (7.40), except that the term involving the derivative of $R_{\pm}(E')$ in the latter equation is missing. In simple scattering problems the magnitude of this third term is of order ϵ times that of the second and vanishes in the limit $\epsilon \to 0$. In quantized field problems, however, this term remains important and is related to the state-vector normalization question. It will be treated further in section 10. For the present we shall drop it from the formalism.

The reactance operator.

A very useful development of the operator formalism in connection with the S-matrix is the introduction of the reactance operator. One uses Eq. (5.28) to split up the terms of Eqs. (7.4) in the following fashion:

$$\left[1 - H_1 \mathcal{P}\frac{1}{E' - H_o}\right] R_\pm(E') = H_1\left[1 \mp \pi i\, \delta(E' - H_o)\, R_\pm(E')\right], \tag{7.47a}$$

$$R_\pm(E')\left[1 - \mathcal{P}\frac{1}{E' - H_o} H_1\right] = \left[1 \mp \pi i\, R_\pm(E')\, \delta(E' - H_o)\right] H_1. \tag{7.47b}$$

These equations then give $R_\pm = K(1 \mp \frac{1}{2} i \underset{\sim}{R}_\pm) = K \mp \frac{1}{2} i R_\pm \underset{\sim}{K}$, or

$$R_\pm = K(1 \pm \tfrac{1}{2} i \underset{\sim}{K})^{-1}, \tag{7.48}$$

$$K = R_\pm(1 \mp \tfrac{1}{2} i \underset{\sim}{R}_\pm)^{-1}, \tag{7.49}$$

where

$$K = \sum{}' K(E')|\zeta_o'\rangle\langle\zeta_o'|, \tag{7.50}$$

$$K(E') = \left[1 - H_1 \mathcal{P}\frac{1}{E' - H_o}\right]^{-1} H_1 = H_1\left[1 - \mathcal{P}\frac{1}{E' - H_o} H_1\right]^{-1} \tag{7.51}$$

$$= H_1\left[1 + \mathcal{P}\frac{1}{E' - H_o} K(E')\right] = \left[1 + K(E')\mathcal{P}\frac{1}{E' - H_o}\right] H_1, \tag{7.52}$$

and where $\underset{\sim}{K}$ is related to K in the same way that the operators $\underset{\sim}{R}_\pm$ are related to $R_\pm$. It is a prevalent figure of speech to refer to the construction of the operators $\underset{\sim}{R}_\pm$, $\underset{\sim}{K}$ from $R_\pm$, K as "taking the matrix elements on the energy shell." Taking the matrix elements of

Eqs. (7.48, 49) on the energy shell, one obtains*

$$\underset{\sim}{R}_{\pm} = \frac{\underset{\sim}{K}}{1 \pm \frac{1}{2} i \underset{\sim}{K}} , \tag{7.53}$$

$$\underset{\sim}{K} = \frac{\underset{\sim}{R}_{\pm}}{1 \mp \frac{1}{2} i \underset{\sim}{R}_{\pm}} . \tag{7.54}$$

$\underset{\sim}{K}$ is known as the reactance operator. It is a real (Hermitian) operator since the operators $K(E')$, by (7.51), are real, and is therefore often easier to construct** in practical cases than the operators $\underset{\sim}{R}_{\pm}$. The latter operators (and hence the S-matrix) can be constructed from $\underset{\sim}{K}$ by solving the integral equation

$$\underset{\sim}{R}_{\pm} = \underset{\sim}{K} \mp \frac{1}{2} i \underset{\sim}{K} \underset{\sim}{R}_{\pm} \tag{7.55}$$

which is known as the <u>Heitler integral equation</u>. [65 to 80] This equation was first introduced in order to describe the effects of radiation damping in field-theoretical scattering problems. How this description comes about can easily be seen by expressing the scattering operator in terms of $\underset{\sim}{K}$. Eqs. (7.44) and (7.53) give

$$S = \frac{1 - \frac{1}{2} i \underset{\sim}{K}}{1 + \frac{1}{2} i \underset{\sim}{K}} P_{J_0} . \tag{7.56}$$

The matrix elements of $\underset{\sim}{K}$ are computed up to a certain order in a perturbation expansion (according to Heitler's original plan, the highest nondiverging order) and then inserted into Eq. (7.56). The presence of $\underset{\sim}{K}$

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* Here one uses the identity $\delta(E'' - E')\,\delta(E''' - E') = \delta(E'' - E''')\,\delta(E''' - E')$.

** The ease of construction shows up particularly when variational techniques are used.

in the denominator insures that many higher terms in the expansion of S are actually included. These higher terms account for the radiation damping and produce a reduction in computed scattering cross sections.

The unitarity of S with respect to the free-state subspace $P_{\mathfrak{J}_0}$ follows directly from Eq. (7.56) and the reality of $\underset{\sim}{K}$. Practical use of Eq. (7.56) has the advantage that S remains unitary even though only an approximation to $\underset{\sim}{K}$ is inserted on the right-hand side.

The phase-shift operator.

Another expression for S which makes its unitarity manifest is the following:

$$S = e^{2i\eta} P_{\mathfrak{J}_0} \tag{7.57}$$

Here η is a real operator known as the phase-shift operator, which is defined only with respect to the subspace $P_{\mathfrak{J}_0}$ and which may be taken to vanish outside it. In terms of η the operators $\underset{\sim}{R}_\pm$ and $\underset{\sim}{K}$ have the forms

$$\underset{\sim}{R}_\pm = -2\, e^{\pm i\eta} \sin\eta \quad , \tag{7.58}$$

$$\underset{\sim}{K} = -2 \tan\eta \quad . \tag{7.59}$$

From Eq. (7.58) one gets

$$\underset{\sim}{R}_\pm^* \underset{\sim}{R}_\pm = \underset{\sim}{R}_\pm \underset{\sim}{R}_\pm^* = 4 \sin^2\eta \tag{7.60}$$

$$= \mp 2\, \mathrm{Im}\, \underset{\sim}{R}_\pm \quad . \tag{7.61}$$

Integral forms.

It is sometimes convenient to introduce integral forms for the operators $R_\pm$, K, $\underset{\sim}{R}_\pm$, $\underset{\sim}{K}$. This may be done by using Eqs. (5.17), (7.8), (7.28) and (2.12), and writing

$$\bar{U}(t, \mp\infty) = P_{\zeta_0} + \sum{}' e^{i(H_0 - E')t} G_{0\pm}(E') R_\pm(E') |\zeta_0'\rangle\langle\zeta_0'|$$

$$= P_{\zeta_0} - i e^{\mp\epsilon t} \sum{}' \int_{\mp\infty}^{t} e^{i(H_0 - E' \mp i\epsilon)t'} R_\pm dt' |\zeta_0'\rangle\langle\zeta_0'|$$

$$\longrightarrow P_{\zeta_0} - i \int_{\mp\infty}^{t} \bar{R}_\pm(t')dt' \tag{7.62}$$

where

$$\bar{R}_\pm(t) = e^{i H_0 t} R_\pm e^{-i H_0 t} . \tag{7.63}$$

Evidently

$$\underset{\sim}{R}_\pm = \int_{-\infty}^{\infty} \bar{R}_\pm(t)dt. \tag{7.64}$$

Using definition (7.63), one gets from Eqs. (5.17) and (7.1)

$$\bar{R}_\pm(t) = \bar{H}_1(t)\, \bar{U}(t, \mp\infty)$$

$$= \bar{H}_1(t) \left[P_{\zeta_0} - i \int_{\mp\infty}^{t} \bar{R}_\pm(t')dt' \right] , \tag{7.65}$$

a result which could also be inferred by substituting (7.62) into the differential equation $i\,\partial\,\bar{U}(t, \mp\infty)/\partial t = \bar{H}_1(t)\,\bar{U}(t, \mp\infty)$.

In a similar manner one may introduce the operator

$$\bar{K}(t) = e^{i H_0 t} K e^{-i H_0 t} \tag{7.66}$$

and use Eq. (7.52) to obtain

$$\bar{K}(t) = \bar{H}_1(t) \left[P_{\zeta_0} + \sum{}' e^{i(H_0 - E')t} \mathcal{P} \frac{1}{E' - H_0} K(E') |\zeta_0'\rangle\langle\zeta_0'| \right]$$

$$= \bar{H}_1(t) \left[P_{\zeta_0} - \tfrac{1}{2} i \sum{}' \int_{-\infty}^{\infty} \sigma(t - t') e^{i(H_0 - E')t' - \epsilon|t - t'|} K\, dt' |\zeta_0'\rangle\langle\zeta_0'| \right]$$

$$\longrightarrow \bar{H}_1(t) \left[P_{\zeta_0} - \tfrac{1}{2} i \int_{-\infty}^{\infty} \sigma(t - t')\, \bar{K}(t')dt' \right] \tag{7.67}$$

where

$$\sigma(t) = t/|t| = \theta_+(t) - \theta_-(t) = 2\,\theta_+(t) - 1 . \tag{7.68}$$

Here we have made use of the integral representation

$$\mathcal{P}\,(1/E) = -\tfrac{1}{2}\,i \int_{-\infty}^{\infty} \sigma(t)\, e^{i\,Et - \epsilon\,|t|}\, dt . \tag{7.69}$$

The relation between the operators $\bar{R}_\pm(t)$ and $\bar{K}(t)$ is determined by Eq. (7.49) to be

$$\bar{R}_\pm(t) = \bar{K}(t)\left[1 \mp \tfrac{1}{2}\,i \int_{-\infty}^{\infty} \bar{R}_\pm(t')dt'\right] , \tag{7.70}$$

which can also be obtained by iterating the split form of Eq. (7.65), namely

$$\bar{R}_\pm(t) = \bar{H}_1(t)\left[P_{\zeta_0} \mp \tfrac{1}{2}\,i \int_{-\infty}^{\infty} \bar{R}_\pm(t')dt' - \tfrac{1}{2}\,i \int_{-\infty}^{\infty} \sigma(t-t')\,\bar{R}_\pm(t')dt'\right] , \tag{7.71}$$

and making a termwise comparison with the iterated form of (7.67). Integration of (7.70) from $-\infty$ to ∞ leads to the Heitler integral equation (7.55), the reactance operator being now expressible as

$$\underset{\sim}{K} = \int_{-\infty}^{\infty} \bar{K}(t)dt . \tag{7.72}$$

<u>Recurrence formulae for $\underset{\sim}{K}$ and S.</u>

When the perturbation H_1 is small enough so that it becomes practicable in actual calculations to compute the operators S and $\underset{\sim}{K}$ by means of series expansions, it is sometimes useful to have available relations between the terms of the two series. The terms themselves may be obtained either by performing a binomial expansion on Eqs. (7.4) and (7.51) or by iterating Eqs. (7.65) and (7.67), and using (7.39). In the latter case one gets

$$S = P_{\mathcal{J}_0} + \sum_{n=1}^{\infty} S_n \quad , \tag{7.73}$$

$$\underset{\sim}{K} = \sum_{n=1}^{\infty} \underset{\sim}{K}_n \quad , \tag{7.74}$$

with

$$S_n = (-i)^n \int_{-\infty}^{\infty} dt_1 \ldots \int_{-\infty}^{\infty} dt_n \, \theta_+(t_1 - t_2) \ldots \theta_+(t_{n-1} - t_n) \bar{H}_1(t_1) \ldots \bar{H}_1(t_n) P_{\mathcal{J}_0} \, , \tag{7.75}$$

$$\underset{\sim}{K}_n = (-\tfrac{1}{2} i)^{n-1} \int_{-\infty}^{\infty} dt_1 \ldots \int_{-\infty}^{\infty} dt_n \, \sigma(t_1 - t_2) \ldots \sigma(t_{n-1} - t_n) \bar{H}_1(t_1) \ldots \bar{H}_1(t_n) P_{\mathcal{J}_0} \, . \tag{7.76}$$

Eq. (7.75) may also be obtained directly from (1.31a), taking $t'' = \infty$, $t' = -\infty$.

If the function $\sigma(t)$ in (7.76) is replaced ny its expression in terms of $\theta_+(t)$ (Eq. (7.63)) and comparison is made with (7.75), one is led to the relations [75]

$$-i \underset{\sim}{K}_n = S_n - \tfrac{1}{2} \sum_{p=1}^{n-1} S_{n-p} S_p + \tfrac{1}{4} \sum_{p=1}^{n-1} \sum_{q=1}^{p-1} S_{n-p} S_{p-q} S_q - \ldots \tag{7.77}$$

$$= S_n \quad \tfrac{1}{2} i \sum_{p=1}^{n-1} S_{n-p} \underset{\sim}{K}_p \tag{7.78a}$$

$$= S_n + \tfrac{1}{2} i \sum_{p=1}^{n-1} \underset{\sim}{K}_p S_{n-p} \quad . \tag{7.78b}$$

Eqs. (7.75 to 78) are especially useful in relativistic field theories, for which covariant calculations are demanded. The first few terms (7.75) of the scattering operator are easily evaluated by standard rules. The corresponding terms of the reactance operator can then be calculated by

means of the recurrence formulae (7.78) and finally substituted back into (7.56) to obtain a unitary S-matrix.

Eqs. (7.78) together with their Hermitian adjoints imply

$$-\underset{\sim}{K}_n = \text{Im } S_n + \tfrac{1}{2} \sum_{p=1}^{n-1} (\text{Re } S_{n-p})\underset{\sim}{K}_p \quad , \tag{7.79}$$

$$0 = \text{Re } S_n - \tfrac{1}{2} \sum_{p=1}^{n-1} (\text{Im } S_{n-p})\underset{\sim}{K}_p \quad , \tag{7.80}$$

since $\underset{\sim}{K}$ is real. Therefore one also has the still more compact formula,

$$\underset{\sim}{K}_n = -\text{Im } S_n - \tfrac{1}{2} \sum_{p+q<n-1} {}_{p,q}(\text{Im } S_{n-p-q})\, \underset{\sim}{K}_p\, \underset{\sim}{K}_q \quad . \tag{7.81}$$

<u>Alternative definition of $\underset{\sim}{K}$.</u>

Heitler [68,69] has invented another method of approach to the reactance operator. He introduces a unitary operator $\overline{W}(t)$ and a transformation

$$\left|\phi(t)\right\rangle = \overline{W}^{-1}(t) \left|\overline{\psi}(t)\right\rangle \tag{7.82}$$

of such a nature that the transformed state-vector satisfies

$$i \frac{d}{dt} \left|\phi(t)\right\rangle = K_1 \left|\phi(t)\right\rangle \tag{7.83}$$

where K_1 is a constant Hermitian operator which is diagonal in energy. Evidently

$$K_1 = \overline{W}^{-1}(t)\, \overline{H}_1(t)\, \overline{W}(t) - i\, \overline{W}^{-1}(t)\, \dot{\overline{W}}(t) \quad . \tag{7.84}$$

Eq. (7.83) describes only <u>real</u> transitions which conserve energy.

If the boundary condition

$$\overline{W}(-\infty) = 1 \tag{7.85}$$

is imposed then Eq. (7.84) may be integrated to give

$$\overline{W}(t) = 1 - i \int_{-\infty}^{t} \left[\overline{H}_1(t') \, \overline{W}(t') - \overline{W}(t') K_1 \right] dt' \, . \tag{7.86}$$

The interesting solution of this equation is the one for which $\overline{W}(t)$ becomes a constant W in the Schrödinger representation, i.e.

$$\overline{W}(t) = e^{i H_0 t} \, W \, e^{-i H_0 t} \, . \tag{7.87}$$

Then

$$\left[W, H_0 \right] = H_1 W - W K_1 \tag{7.88}$$

and

$$W P_{\zeta_0} = P_{\zeta_0} - i \sum{}' \int_{-\infty}^{0} e^{i(H_0 - E')t'} \left(H_1 W - W K_1 \right) dt' \, |\zeta_0'\rangle\langle\zeta_0'|$$

$$\longleftarrow \sum{}' W(E') \, |\zeta_0'\rangle\langle\zeta_0'| \, , \tag{7.89}$$

where

$$\begin{aligned} W(E') &= 1 + G_{0+}(E') \left[H_1 W(E') - W(E') K_1 \right] \\ &= \left[1 - G_{0+}(E') H_1 \right]^{-1} \left[1 - W(E') K_1 \right] \, . \end{aligned} \tag{7.90}$$

Now, the matrix elements of (7.88) which are diagonal in energy vanish. Therefore, by (7.86),

$$\overline{W}(\infty) = 1 - i \sum{}' \int_{-\infty}^{\infty} e^{i(H_0 - E')t} (H_1 W - W K_1) dt \, |\zeta_0'\rangle\langle\zeta_0'| = 1 \, , \tag{7.91}$$

and hence, with (7.85),

$$|\phi(\pm\infty)\rangle = |\overline{\psi}(\pm\infty)\rangle \, . \tag{7.92}$$

This means that the scattering operator may be constructed from K_1 in exactly the same manner as it is constructed from H_1. That is,

$$\bar{U}(\pm\infty, \mp\infty) = P_{\zeta_0} \mp 2\pi i \sum{}' \delta(E' - H_0)\, K_1 \left[1 - G_{0\pm}(E')K_1\right]^{-1} |\zeta_0'\rangle\langle\zeta_0'|$$

$$= P_{\zeta_0} \mp i \underset{\sim}{K}_1 \left[1 - K_1/(\pm i\epsilon)\right]^{-1} . \tag{7.93}$$

But since K_1 is diagonal in energy

$$\underset{\sim}{K}_1 = \sum{}' \frac{2\epsilon}{(E' - H_0)^2 + \epsilon^2} K_1 |\zeta_0'\rangle\langle\zeta_0'| = (2K_1/\epsilon) P_{\zeta_0} , \tag{7.94}$$

so that (7.93) becomes

$$\bar{U}(\pm\infty, \mp\infty) = P_{\zeta_0} \mp i \underset{\sim}{K}_1 (1 \pm \tfrac{1}{2} i \underset{\sim}{K}_1)^{-1} \tag{7.95}$$

which leads to the identification*

$$\underset{\sim}{K} = \underset{\sim}{K}_1 . \tag{7.96}$$

The operator $W P_{\zeta_0}$ may now be constructed by iteration of (7.90):

$$W P_{\zeta_0} = \sum{}' \sum_{n=0}^{\infty} (-1)^n \left[1 - G_{0+}(E')H_1\right]^{-(n+1)} (\tfrac{1}{2}\epsilon \underset{\sim}{K})^n |\zeta_0'\rangle\langle\zeta_0'| . \tag{7.97}$$

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* The same result is obtained by writing

$$\underset{\sim}{K} = 2\pi \sum{}' \delta(E' - H_0) K_1 \left[1 - \mathcal{P}\frac{1}{E' - H_0} K_1\right]^{-1} |\zeta_0'\rangle\langle\zeta_0'|$$

and remembering that $\mathcal{P}\, 1/(E' - E'')$ vanishes for $E'' = E'$.

Heitler bases his construction of the operators W and K_1 (and hence of $\underset{\sim}{K}$) directly on Eq. (7.88) plus the conditions that W be unitary and that K_1 be diagonal in energy. As this construction is rather complicated, however, we omit it here and refer the reader to the reference cited earlier.

8. CROSS SECTIONS

Return to the wave packet picture.

In the preceding three sections emphasis has been placed on the operators $\bar{U}(0, \mp\infty)$, $\bar{U}(\pm\infty, \mp\infty)$, etc. as abstract formal entities more or less independent of any immediate physical processes. It is to be remembered, however, that the limiting procedure of adiabatic switching and the related limiting convention (5.22), which were adopted in order to give precise definitions to these operators, were motivated by physical considerations. In fact, an "operational" definition of these operators within the context of a given physical situation is always possible and sometimes preferable. Thus, if the scattering of wave packets is under consideration one may validly write

$$\bar{U}(t, -\infty)\,|\,\text{in}\rangle \equiv \lim_{t' \to -\infty} \bar{U}(t, t')\,|\,\text{in}\rangle \tag{8.1}$$

where $|\text{in}\rangle$ specifies the incoming wave packet of (4.5) and the limit $t' \to -\infty$ is to be taken perfectly straightforwardly, although the equation is meaningless if the vector $|\text{in}\rangle$ is omitted. The presence of the vector $|\text{in}\rangle$ provides the physical context, and the equation says simply that $\bar{U}(t, -\infty)\,|\,\text{in}\rangle$ may be regarded by definition as the result of bringing the wave packet into the picture at an unspecified time in the sufficiently remote past.

In the derivation of the basic cross section formulae in the theory of scattering the use of operational definitions involving wave packets is particularly appropriate. To be sure, several derivations of these formulae exist [30,42,160] which proceed directly from expressions for the abstract entities $\bar{U}(t, \mp\infty)$, $\bar{U}(\pm\infty, \mp\infty)$ themselves, via more or less obscure arguments.

Wave packet derivations, however, stay closer to experimental reality and are therefore both more physically satisfactory and more correct. These latter are the derivations which will be presented in this article.

Before turning to the cross section formulae it is instructive to verify directly the existence of the limit in (8.1). In so doing one will be led to a more concise if not more rigorous proof of Eq. (4.30), the derivation of which in section 4 depended upon picturesque but somewhat loose arguments involving the qualitative behavior of retarded and advanced waves. The following formal identity will be needed:

$$\lim_{t \to \pm\infty} \mathcal{P}(e^{iEt}/E) \equiv \pm \pi i \delta(E) . \tag{8.2}$$

This is to be understood, as usual, as an abbreviation for a class of integral identities. Its derivation is brief:

$$\lim_{t \to \pm\infty} \mathcal{P}\int_{-\infty}^{\infty} (e^{iEt}/E) f(E) dE = \lim_{t \to \pm\infty} \mathcal{P}\int_{\mp\infty}^{\pm\infty} (e^{ix}/x)\, f(x/t) dx$$

$$= \pm \pi i\, f(0) \tag{8.3}$$

where $x = Et$.

Now consider the vector $\bar{U}(0, t)|\zeta_0'\rangle = e^{i(H-E')t}|\zeta_0'\rangle$. Expand $|\zeta_0'\rangle$ in terms of the eigenvectors of the operator H and use Eqs. (7.7) and (5.28), getting [43]

$$\bar{U}(0, t)|\zeta_0'\rangle = |\zeta_\pm'\rangle + \sum{}'' e^{i(E''-E')t} |\zeta_0''\rangle \langle\zeta_0''|H_1 G_{0\mp}(E'')|\zeta_0'\rangle$$

$$+ \sum{}'' e^{i(H''-E')t} |J''\rangle\langle J''|\zeta_0'\rangle$$

(continued on next page)

$$= |\zeta_\pm'\rangle \pm \pi i \sum{}'' \delta(E'' - E') |\zeta_\pm''\rangle\langle\zeta_\pm''|H_1|\zeta_0'\rangle$$

$$+ \mathcal{P} \sum{}'' \frac{e^{i(E'' - E')t}}{E'' - E'} |\zeta_\pm''\rangle\langle\zeta_\pm''|H_1|\zeta_0'\rangle$$

$$+ \sum{}'' \frac{e^{i(H'' - E')t}}{H'' - E'} |J''\rangle\langle J''|H_1|\zeta_0'\rangle \quad . \tag{8.4}$$

In the last line the identity

$$\langle J''|H_1|\zeta_0'\rangle = \langle J''|(H - H_0)|\zeta_0'\rangle = (H'' - E')\langle J''|\zeta_0'\rangle \tag{8.5}$$

has been used. Next, sum Eq. (8.4) over the wave packet amplitudes of Eq. (4.5) and then pass to the limit $t \to -\infty$, obtaining, with the use of (8.2),

$$\lim_{t\to-\infty} \bar{U}(0, t)|in\rangle$$

$$= \sum{}' f(\zeta_0')|\zeta_\pm'\rangle - \pi i(1 \mp i)\sum{}' \sum{}'' f(\zeta_0')\delta(E'' - E')|\zeta_\pm''\rangle\langle\zeta_\pm''|H_1|\zeta_0'\rangle$$

$$- \pi i \sum{}' \sum{}'' f(\zeta_0')\delta(H'' - E')|J''\rangle\langle J''|H_1|\zeta_0'\rangle \quad . \tag{8.6}$$

The last term vanishes since the bound state spectrum does not overlap the continuous spectrum. It is to be noted that the use of (8.2) in obtaining the factor $\delta(H'' - E')$ in this term is justified only <u>after</u> the packet summation is performed, for only then does the rapidly varying exponential appear in an integral, viz. the summation over the continuous range of energies E' contained in the packet. On the other hand, the use of (8.2)

to obtain the factor $\delta(E'' - E')$ in the second term is permitted before the packet summation. This means that if H has no bound states the use of a wave packet is not actually mandatory in defining the matrix elements of $\bar{U}(0, -\infty)$. The limit as $t \to -\infty$ of $\bar{U}(0, t)|\zeta_0'\rangle$ will in this special case exist independently in its own right and be identical with the result of the limiting convention (5.22).

If the $|\zeta_+'\rangle$ are chosen as basic vectors in Eq. (8.6) then the second term on the right also vanishes, leaving nothing but the first term which is simply the vector $|\underset{\sim}{\psi}\rangle$ defined by (4.3). In the limit of a very broad packet therefore one is led to Eq. (4.30) as predicted. The choice of the $|\zeta_-'\rangle$ as basic vectors, on the other hand, yields together with (4.30) the result

$$|\zeta_+'\rangle = |\zeta_-'\rangle - 2\pi i \sum{}'' \delta(E'' - E')|\zeta_-''\rangle\langle\zeta_0''| \; R_+ |\zeta_0'\rangle , \tag{8.7}$$

which, when multiplied on the left by $\langle\zeta_-''|$, leads to expression (7.40) for the S-matrix (with the derivative term omitted).

When t in Eq. (8.1) is not restricted to the value zero, one has the more general result

$$\bar{U}(t, -\infty)|in\rangle = e^{iH_0 t} e^{-iHt} |\underset{\sim}{\psi}\rangle . \tag{8.8}$$

Multiplication of this equation on the left by $\langle\zeta_0''|$ and use of (4.3), (7.7) and (5.28) gives

$$\langle\zeta_0''|\bar{U}(t, -\infty)|in\rangle = \sum{}' f(\zeta_0') e^{i(E'' - E')t} \langle\zeta_0''|\zeta_+'\rangle$$

$$= f(\zeta_0'') - \pi i \sum{}' f(\zeta_0')\delta(E'' - E')\langle\zeta_0''|H_1|\zeta_+'\rangle$$

$$- \mathcal{P} \sum{}' f(\zeta_0') \frac{e^{i(E'' - E')t}}{E'' - E'} \langle\zeta_0''|H_1|\zeta_+'\rangle . \tag{8.9}$$

Allowing t to become infinite, using (8.2), and then allowing the packet to become very broad,* one obtains again expression (7.40) for the S-matrix. This is sometimes regarded as an alternative demonstration of the equivalence of the time-dependent and time-independent definitions of the S-matrix (Eq. (4.28)).

Transition rates and the angular cross section.

The cross section formulae can be derived by two independent arguments, one based on the computation of transition rates and the other based directly on the S-matrix. We present the transition-rate argument first.

If the system H is known to be in the incoming packet state which, in the remote past, is described by the interaction state vector $|\text{in}\rangle$, the probability of finding it in the state $|\zeta_0''\rangle$ at the time t is given (see Eq.(1.42)) by

$$P(\zeta_0'', t \,|\, \text{in}, -\infty) = \left|\langle \zeta_0'' | \bar{U}(t, -\infty) | \text{in}\rangle\right|^2$$
$$= \left|\langle \zeta_0'' | e^{i H_0 t} e^{-i H t} | \underset{\sim}{\psi}\rangle\right|^2 . \tag{8.10}$$

The rate of transition to the state $|\zeta_0''\rangle$ is the time derivative of this quantity:

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* It should be clear that the procedure of passing to the limit $\epsilon \to 0$ at the end of a derivation played the same analytic role in previous sections as the final passage to a very broad packet plays in the derivations of the present section. Use of a finite ϵ avoids the necessity for dealing with finite wave packets, and vice versa. The two methods are not, however, equivalent in physical detail as some authors [30, 160] have assumed.

$$R(\zeta_0'' \mid \text{in}) = \frac{d}{dt} P(\zeta_0'', t \mid \text{in}, -\infty)$$

$$= -2\,\mathrm{Im}\left[\langle \underset{\sim}{\psi} | e^{iHt} H_1 e^{-iH_0 t} | \zeta_0'' \rangle \langle \zeta_0'' | e^{iH_0 t} e^{-iHt} | \underset{\sim}{\psi} \rangle\right]. \tag{8.11}$$

In the limit of a very broad packet this expression reduces to

$$R(\zeta_0'' \mid \zeta_0') = -2\,\mathrm{Im}\left[\langle \zeta_+' | H_1 | \zeta_0'' \rangle \langle \zeta_0'' | \zeta_+' \rangle\right]$$

$$= -2\,\mathrm{Im}\left\{\langle \zeta_0' | R_-(E') | \zeta_0'' \rangle \left[\delta(\zeta_0'', \zeta_0') + \langle \zeta_0'' | G_{0+}(E') R_+(E') | \zeta_0' \rangle\right]\right\}$$

$$= 2\,\delta(\zeta_0'', \zeta_0')\,\mathrm{Im}\,\langle \zeta_0' | R_+ | \zeta_0' \rangle + 2\pi\,\delta(E'' - E') \left|\langle \zeta_0'' | R_+ | \zeta_0' \rangle\right|^2 \tag{8.12}$$

which is <u>independent of the time</u>.

Now suppose that the unperturbed Hamiltonian H_0 is a function only of the absolute value of the N-dimensional momentum vector $\underset{\sim}{p}$ of the scattered particle.* This vector will then be a constant of the motion of the comparison system, permitting the labels ζ_0' to be chosen as $\underset{\sim}{p}'$, σ', where σ' describes any internal or nonclassical degrees of freedom which the particle or scatterer may have. The velocity of the particle in the state $|\underset{\sim}{p}', \sigma'\rangle$ will be given by

$$v' = dE'/dp' \tag{8.13}$$

where $p' = |\underset{\sim}{p}'|$. The state vector $|\underset{\sim}{p}', \sigma'\rangle$ evidently corresponds to a particle flux density of $v'L^{-N}$, and therefore the angular cross section $\sigma(\underset{\sim}{\Omega}, \sigma'' \mid \underset{\sim}{p}', \sigma')$ describing scattering from an initial very

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* The method of handling the more general case will be indicated in section 12 where scattering by two or more potentials is discussed.

broad packet, which has $|\underset{\sim}{p}', \sigma'\rangle$ as its limiting form, into a final state with momentum directed along a unit vector $\underset{\sim}{\Omega}$ and with nonclassical degrees of freedom as indicated, is defined by

$$v' L^{-N} \sigma(\underset{\sim}{\Omega}, \sigma'' | \underset{\sim}{p}', \sigma') d^{N-1}\underset{\sim}{\Omega} = \sum_{\underset{\sim}{p}'' \text{ in } d^{N-1}\underset{\sim}{\Omega}} R(\underset{\sim}{p}'', \sigma'' | \underset{\sim}{p}', \sigma') . \tag{8.14}$$

Here $d^{N-1}\underset{\sim}{\Omega}$ is the (N-1)-dimensional element of solid angle in the direction $\underset{\sim}{\Omega}$. (If $N = 1$ then $d^0\underset{\sim}{\Omega} = 1$ and integration over solid angle reduces to a summation over the two possible values of $\underset{\sim}{\Omega}$, $+1$ and -1.)

When the system is placed in the rectangular box of side L, the element of momentum space becomes

$$d^N \underset{\sim}{p}'' = (2\pi/L)^N , \tag{8.15}$$

and the summation $\sum_{\underset{\sim}{p}''}$ in (8.14) may be replaced by $(L/2\pi)^N \int d^N \underset{\sim}{p}''$. One may further write

$$d^N \underset{\sim}{p}'' = dE'' \, d^{N-1}\underset{\sim}{\Omega} \, \partial(\underset{\sim}{p}'')/\partial(E'', \underset{\sim}{\Omega}'') \tag{8.16}$$

where

$$\partial(\underset{\sim}{p}'')/\partial(E'', \underset{\sim}{\Omega}'') = (dp''/dE'')\,\partial(\underset{\sim}{p}'')/\partial(p'', \underset{\sim}{\Omega}'')$$

$$= p''^{N-1}/v'' . \tag{8.17}$$

Consider now the case in which $\underset{\sim}{p}'$ does not lie in $d^{N-1}\underset{\sim}{\Omega}$. Then, introducing the operator

$$\mathcal{R}_+ = L^N R_+ \tag{8.18}$$

in order to work with finite quantities, one may insert (8.12) into (8.14) and use (8.16, 17), obtaining

$$\sigma(\underset{\sim}{\Omega}, \sigma'' \mid \underset{\sim}{p}', \sigma')$$

$$= 2\pi(L^N/v')(L/2\pi)^N L^{-2N} \int dE''(p''^{N-1}/v'')\,\delta(E'' - E')$$

$$\times \left|\left\langle p''\underset{\sim}{\Omega}, \sigma'' \middle| \mathfrak{R}_+ \middle| \underset{\sim}{p}', \sigma' \right\rangle\right|^2$$

$$= (2\pi)^{-(N-1)}(p'^{N-1}/v'^2) \left|\left\langle p'\underset{\sim}{\Omega}, \sigma'' \middle| \mathfrak{R}_+ \middle| \underset{\sim}{p}', \sigma' \right\rangle\right|^2 . \tag{8.19}$$

<u>Derivation based on the S-matrix.</u>

Here it is convenient to specify the wave packet in slightly greater detail. We shall use an incoming packet which has the form of a plane slab of area L^{N-1}:*

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* Here we assume the enclosing box to be oriented so that one of its axes is parallel to $\underset{\sim}{p}'$.
The generalization to the case of a packet of smaller area is easy. The packet must, however, always be broader than and aimed at the scattering region. Typically in an actual experiment the lateral breadth Δx_l is given by the aperture diameter of the beam collimator. This implies an uncertainty in lateral momentum of amount $\approx 1/\Delta x_l$ and hence a lateral velocity spread roughly equal to $v'/(p'\Delta x_l)$. In order that the results of the present section be applicable to experiment the lateral spreading of the packet must be negligible ($\ll \Delta x_l$) during the transit time l/v', where l is the distance from the collimator to the detector of the scattered beam. The following inequality must therefore be satisfied: $p' \gg l/(\Delta x_l)^2$. It is easily verified, by the insertion of actual numbers, that with typical laboratory dimensions, energies and accuracies this inequality is satisfied for all molecules and atoms and all elementary particles except very soft photons and neutrinos (<1 eV.).

$$\left|\text{in}\right\rangle = \left|\bar{\psi}(-\infty)\right\rangle = \int f(p''')\left|p'''\underset{\sim}{\Omega}', \sigma'\right\rangle dp''' . \tag{8.20}$$

Here $f(p''')$ is a function which is peaked around the value p' with a spread which will be denoted by Δp. It will be assumed that the experimental apparatus has provided a sufficiently monoenergetic particle beam so that $f(p''')$ varies much more rapidly with p''' than do the elements of the S-matrix. That is, Δp is so small that $\left|f(p''')\right|^2$ is virtually a delta function as far as integration over these matrix elements is concerned.

The vector $\left|\text{in}\right\rangle$ is conveniently normalized to unit probability per unit area of the incoming slab. This means

$$L^{N-1} = \left\langle \text{in}\middle|\text{in}\right\rangle = (2\pi/L)\int \left|f(p''')\right|^2 dp''' , \tag{8.21}$$

in which the relation $dp''' = 2\pi/L$ has been used. With this normalization the scattering cross section is given directly by the amount of "probability" scattered out of the slab. The components of the scattered state vector are

$$\begin{aligned}\left\langle \underset{\sim}{p}'', \sigma''\middle|\text{out}\right\rangle &= \left\langle \underset{\sim}{p}'', \sigma''\middle|\bar{\psi}(\infty)\right\rangle = \left\langle \underset{\sim}{p}'', \sigma''\middle|S\middle|\text{in}\right\rangle \\ &= -2\pi i\int f(p''')\,\delta(E''-E''')\left\langle \underset{\sim}{p}'', \sigma''\middle| R_+\middle|p'''\underset{\sim}{\Omega}', \sigma'\right\rangle dp''' \\ &= -L^{-N}(2\pi i/v'')\, f(p'')\left\langle \underset{\sim}{p}'', \sigma''\middle|\mathcal{R}_+\middle| p''\underset{\sim}{\Omega}', \sigma'\right\rangle\end{aligned} \tag{8.22}$$

when $\underset{\sim}{p}''$ is not parallel to $\underset{\sim}{\Omega}'$, and hence the angular cross section is given by

$$\begin{aligned}\sigma(\underset{\sim}{\Omega}, \sigma''\,|\,\underset{\sim}{p}', \sigma')\, d^{N-1}\underset{\sim}{\Omega} &= \sum_{p''\ \text{in}\ d^{N-1}\underset{\sim}{\Omega}} \left|\left\langle \underset{\sim}{p}'', \sigma''\middle|\ \text{out}\right\rangle\right|^2 \\ &= (L/2\pi)^N L^{-2N}\, d^{N-1}\underset{\sim}{\Omega}\int (2\pi/v'')^2\, p''^{N-1}\left|f(p'')\right|^2 \left|\left\langle \underset{\sim}{p}'', \sigma''\middle|\mathcal{R}_+\middle| p''\underset{\sim}{\Omega}', \sigma'\right\rangle\right|^2 dp'' ,\end{aligned} \tag{8.23}$$

leading, in virtue of (8.21) and the delta function character of $|f(p'')|^2$, to Eq. (8.19).

The connection between transition rates and the S-matrix.

The existence of the preceding two independent derivations of the angular cross section formula (8.19) implies a direct connection between the transition rate (8.12) and the S-matrix. This connection follows, in fact, from the time independence of the transition rate in the limit of a very broad incident packet, which allows the total probability of transition from the state $|\zeta_0'\rangle$ at $t = -\infty$ to the state $|\zeta_0''\rangle$ at $t = \infty$ to be expressed in the form

$$P(\zeta_0'', \infty \mid \zeta_0', -\infty) = \delta(\zeta_0'', \zeta_0') + \int_{-\infty}^{\infty} R(\zeta_0'' \mid \zeta_0')dt$$

$$= \delta(\zeta_0'', \zeta_0')\left[1 + 2T' \operatorname{Im} \langle \zeta_0' | R_+ | \zeta_0' \rangle\right] + 2\pi T' \delta(E'' - E') \left| \langle \zeta_0'' | R_+ | \zeta_0' \rangle \right|^2, \tag{8.24}$$

where T' is a purely formal symbol which is used to replace the expression $\int_{-\infty}^{\infty} dt$. Now, setting $t = \infty$ and $|\text{in}\rangle = |\zeta_0'\rangle$ in (8.10), one may also write

$$P(\zeta_0'', \infty \mid \zeta_0', -\infty) = \left| \langle \zeta_0'' | S | \zeta_0' \rangle \right|^2 . \tag{8.25}$$

Eqs. (8.24) and (8.25) agree with expression (7.40) for the S-matrix provided a convention is adopted which is expressed in the formal equation

$$\delta(E'' - E') = (T'/2\pi)\delta_{E''E'} , \tag{8.26}$$

which may be compared with Eq. (5.30). This convention is sometimes used without refinement to "derive" the transition rate, and hence the cross sections, directly from the S-matrix. One simply divides Eq. (8.25) by T'.

A question naturally arises as to the extent of the applicability of the formal equation (8.26) as an ordinary algebraic equation. This question becomes especially pertinent when it is remembered that the delta function, in the formalism of all preceding sections, is regarded as the limiting form of a function (5.27) which has a finite half width ϵ. Since condition (7.18) must always hold, the distribution of states $|\mathfrak{I}_0'\rangle$ is always fine-grained with respect to this width. Hence the limiting behavior of $\delta(E'' - E')$ is <u>not</u> as indicated by (8.26) in which it vanishes unless the levels E'' and E' are identical. The "energy shell" embraced by $\delta(E'' - E')$ contains, in the limit, an infinitesimally thin but <u>infinite</u> group of levels rather than merely a single level. The replacement of the delta function by a weight factor times the Kronecker delta can therefore be permitted only if the factors which multiply it in any summand or integrand vary slowly across the energy shell while ϵ is still finite.

That this condition usually holds may be seen by examining one or two special cases. An example which affords a certain amount of insight is provided by the wave packet integration of Eq. (8.22). If the delta function in this equation is replaced by a function with a finite half width ϵ it is necessary to remember that this replacement corresponds to a physical complication of the scattering process consisting of an adiabatic switching procedure having a time duration of $2/\epsilon$. In order that the actual scattering picture remain unchanged the wave packet must pass completely through the scattering region while the perturbation H_1 is essentially at full strength. Assuming the dimensions of the scattering region to be much smaller than those of the packet, this requires that $\Delta x/v' \ll 2/\epsilon$, where Δx is the thickness of the packet. But

since $\Delta x \gtrsim 1/\Delta p$ this means $\Delta E = v'\Delta p \gg \epsilon/2$. That is, the energy spread of the packet must be much broader than the function having the half width ϵ, so that the latter is still an effective delta function in the equation. Said in another way, $f(p''')$ must have negligible variation across the energy shell.

Similar conclusions hold for the factors multiplying $\delta(E'' - E')$ in expressions of the form

$$\underset{\sim}{F} = 2\pi \sum{}' \sum{}'' \delta(E'' - E') \left|\zeta_0''\right\rangle \left\langle \zeta_0'' \right| F \left|\zeta_0'\right\rangle \left\langle \zeta_0' \right|$$

where $F = R_\pm, K$. Here, although $R_\pm$ and K depend on ϵ, they approach their limits smoothly as $\epsilon \to 0$. Furthermore, the matrix elements of these limits generally vary smoothly, allowing ϵ to be chosen small enough so that this variation becomes negligible across the energy shell. Eq. (8.26) may therefore be validly applied to the process of taking matrix elements of given operators on the energy shell, and one may conveniently write

$$\left\langle \zeta_0'' \right| \underset{\sim}{F} \left| \zeta_0' \right\rangle = T' \delta_{E''E'} \left\langle \zeta_0'' \right| F \left| \zeta_0' \right\rangle . \tag{8.27}$$

An exception to the rule (8.27) is provided by the operator K_1 introduced at the end of section 7. It would not be correct to infer from Eqs. (7.94) and (8.27) the identity $T' = 2/\epsilon$. Eq. (8.27) cannot be applied in this case simply because K_1 is already diagonal in energy, and hence its matrix elements always vary abruptly across the energy shell. That $T' \neq 2/\epsilon$ can be seen from the formal identity

$$\delta_{E''E'} = \delta(E'' - E')dE' = \delta(E'' - E')v' \, dp' . \tag{8.28}$$

Combining this with (8.26) and using the equation $dp' = 2\pi/L$, one obtains the formal relation

$$T' = L/v' . \tag{8.29}$$

That is, T' may be regarded as the length of time required for the incident particle to traverse the enclosing box, and in virtue of condition (7.18) this implies $T' \gg 2/\epsilon$.

In the future we shall not hesitate, if convenient, to use the T-symbol as an ordinary algebraic quantity. It is always to be remembered, however, that it is a purely formal weight factor which will cancel out in the final expression for any physically observable quantity.

The total cross section.

It is customary to define the angular cross section by Eq. (8.19) even when $\underset{\sim}{p}'$ is parallel to $\underset{\sim}{\Omega}$. However, the true depletion in the forward direction of a beam of incoming particles (or packets) is described not by this quantity but by the total scattering cross section, which, in the transition rate argument, is defined by

$$\begin{aligned}\sigma(\underset{\sim}{p}', \sigma') &= -(L^N/v') \sum_{\underset{\sim}{p}''} R(p''\underset{\sim}{\Omega}', \sigma' \mid \underset{\sim}{p}', \sigma') \\ &= -(2/v') \operatorname{Im} \langle \underset{\sim}{p}', \sigma' | \mathcal{R}_+ | \underset{\sim}{p}', \sigma' \rangle \\ &\quad -(L^{-(N-1)}/v'^2) \left| \langle \underset{\sim}{p}', \sigma' | \mathcal{R}_+ | \underset{\sim}{p}', \sigma' \rangle \right|^2 ,\end{aligned} \tag{8.30}$$

where use has been made of the relation $\sum_{p''} F(p'') \, \delta(E'' - E') = (L/2\pi v') F(p')$.* In the argument based directly on the S-matrix, using a finite slab for a packet, the forward depletion is defined by

$$\begin{aligned}\sigma(\underset{\sim}{p}', \sigma') &= \langle \text{in} | \text{in} \rangle - \sum_{p''} \left| \langle p''\underset{\sim}{\Omega}', \sigma' | \text{out} \rangle \right|^2 \\ &= L^{N-1} - (2\pi/L) \int dp'' \, |f(p'')|^2 \Big[1 + 2(L^{-(N-1)}/v'') \operatorname{Im} \langle p''\underset{\sim}{\Omega}', \sigma' | \mathcal{R}_+ | p''\underset{\sim}{\Omega}', \sigma' \rangle \\ &\qquad + (L^{-(N-1)}/v'')^2 \left| \langle p''\underset{\sim}{\Omega}', \sigma' | \mathcal{R}_+ | p''\underset{\sim}{\Omega}', \sigma' \rangle \right|^2 \Big] ,\end{aligned} \tag{8.31}$$

* Here again we assume $\underset{\sim}{p}'$ is parallel to one of the box axes.

which also yields the same result. In passing from the first to the second line of Eq. (8.31) it is necessary to use the generalization of Eq. (8.22) which takes into account diagonal elements of the S-matrix:

$$\left\langle p''\underset{\sim}{\Omega}', \sigma' \middle| \text{out} \right\rangle = \int f(p''') \left\langle p''\underset{\sim}{\Omega}', \sigma' \middle| S \middle| p'''\underset{\sim}{\Omega}', \sigma' \right\rangle dp'''$$

$$= f(p'') \left[(2\pi/L) - L^{-N}(2\pi i/v'') \left\langle p''\underset{\sim}{\Omega}', \sigma' \middle| \mathcal{R}_+ \middle| p''\underset{\sim}{\Omega}', \sigma' \right\rangle \right]. \tag{8.32}$$

A distinction is immediately apparent between the cases $N = 1$ and $N \geqslant 2$. In the latter case the last term of Eq. (8.30) vanishes in the limit $L \to \infty$, and the total cross section is seen to be determined completely by the imaginary part of the amplitude for forward scattering with no change in the variables σ'.

For $N \geqslant 2$ the relation between the total and angular cross sections may be readily obtained by using Eq. (7.61) of the last section. Taking the diagonal elements of this equation, using (8.26), and removing a factor $T'L^{-N}$ from both sides, one gets

$$-2\,\mathrm{Im}\left\langle \underset{\sim}{p}', \sigma' \middle| \mathcal{R}_+ \middle| \underset{\sim}{p}', \sigma' \right\rangle = 2\pi L^{-N} \sum{}'' \delta(E'' - E') \left| \left\langle \underset{\sim}{p}'', \sigma'' \middle| \mathcal{R}_+ \middle| \underset{\sim}{p}', \sigma' \right\rangle \right|^2, \tag{8.33}$$

which implies

$$\sigma(\underset{\sim}{p}', \sigma') = \sum_{\sigma''} \int \sigma(\underset{\sim}{\Omega}, \sigma'' \,|\, \underset{\sim}{p}', \sigma') d^{N-1}\underset{\sim}{\Omega}. \tag{8.34}$$

Eqs. (8.33, 34) are consequences of the unitarity of the scattering operator with respect to the free states $\left| \underset{\sim}{p}', \sigma' \right\rangle$, and are simple expressions of the conservation of probability.

<u>The case $N = 1$. Transmission and reflection coefficients.</u>

In the one-dimensional case the cross sections become dimensionless probabilities and are conveniently replaced by the so-called <u>transmission</u>

and reflection coefficients, $T_{\sigma''\sigma'}$ and $R_{\sigma''\sigma'}$ respectively. The diagonal transmission coefficient $T_{\sigma'\sigma'}$ is defined as unity minus the forward depletion:

$$T_{\sigma'\sigma'}(\underset{\sim}{p}') = 1 + (2/v') \operatorname{Im} \langle \underset{\sim}{p}', \sigma' | \mathcal{R}_+ | p', \sigma' \rangle + (1/v'^2) \left| \langle \underset{\sim}{p}', \sigma' | \mathcal{R}_+ | \underset{\sim}{p}', \sigma' \rangle \right|^2 . \tag{8.35}$$

The other coefficients have the definitions

$$T_{\sigma''\sigma'}(\underset{\sim}{p}') = \sigma(\underset{\sim}{\Omega}', \sigma'' | \underset{\sim}{p}', \sigma'), \qquad \sigma'' \neq \sigma' , \tag{8.36}$$

$$R_{\sigma''\sigma'}(\underset{\sim}{p}') = \sigma(-\underset{\sim}{\Omega}', \sigma'' | \underset{\sim}{p}', \sigma'). \tag{8.37}$$

Conservation of probability has in this case the expression

$$\sum\nolimits_{\sigma''} \left[T_{\sigma''\sigma'}(\underset{\sim}{p}') + R_{\sigma''\sigma'}(\underset{\sim}{p}') \right] = 1 \qquad \text{for all } \underset{\sim}{p}', \sigma' . \tag{8.38}$$

The transmission and reflection coefficients may be directly related to the total transition probabilities from $t = -\infty$ to $t = \infty$. Using (8.18), (8.26) and (8.29) in Eq. (8.24), one readily sees that

$$T_{\sigma''\sigma'}(\underset{\sim}{p}') = P(\underset{\sim}{p}', \sigma'', \infty | \underset{\sim}{p}', \sigma', -\infty), \tag{8.39}$$

$$R_{\sigma''\sigma'}(\underset{\sim}{p}') = P(-\underset{\sim}{p}', \sigma'', \infty | \underset{\sim}{p}', \sigma', -\infty). \tag{8.40}$$

Phase shift formulae.

In many practical applications it is useful to discuss scattering in terms of the phase shift operator η. η is an Hermitian operator and hence can always be diagonalized in principle. It is already diagonal with respect to energy. Denote by λ' the remaining labels necessary to complete the diagonalization process:

$$\langle E'', \lambda'' | \eta | E', \lambda' \rangle = \delta_{E''E'} \delta_{\lambda''\lambda'} \eta' \quad . \tag{8.41}$$

The expansion of the vectors $|\underset{\sim}{p}', \sigma'\rangle$ in terms of $|E', \lambda'\rangle$ will be needed:

$$\langle \underset{\sim}{p}'', \sigma'' | E', \lambda' \rangle = C' \, \delta_{E''E'} \, \mathcal{Y}_{\lambda'}(E', \underset{\sim}{\Omega}'', \sigma'') . \tag{8.42}$$

Here the $\mathcal{Y}_{\lambda'}$ are functions normalized on the unit N-dimensional sphere.

$$\sum_{\sigma''} \int \mathcal{Y}_{\lambda''}{}^{*}(E', \underset{\sim}{\Omega}'', \sigma'') \, \mathcal{Y}_{\lambda'}(E', \underset{\sim}{\Omega}'', \sigma'') d^{N-1}\underset{\sim}{\Omega}'' = \delta_{\lambda''\lambda'} . \tag{8.43}$$

The normalization constant C' is chosen so that

$$\sum{}''' \langle E'', \lambda'' | \underset{\sim}{p}''', \sigma''' \rangle \langle \underset{\sim}{p}''', \sigma''' | E', \lambda' \rangle = \delta_{E''E'} \delta_{\lambda''\lambda'} . \tag{8.44}$$

Inserting (8.42) into the left side of this equation, and using Eqs. (8.15), (8.26) and (8.43), one finds

$$C' = (T'/2\pi)^{\frac{1}{2}} (2\pi/L)^{N/2} (v'/p'^{N-1})^{\frac{1}{2}} . \tag{8.45}$$

If now $2\pi\delta(E'' - E')$ is replaced by $T'\delta_{E''E'}$ in Eq. (7.45) which defines the operator $\underset{\sim}{R}_+$, and if Eq. (7.58) which expresses this operator in terms of η is used, then the cross section formula (8.19) becomes

$$\begin{aligned}
&\sigma(\underset{\sim}{\Omega}, \sigma'' | \underset{\sim}{p}', \sigma') \\
&= (2\pi)^{-(N-1)} (p'^{N-1}/v'^{2}) T'^{-2} L^{2N} \left| \sum_{\lambda'} \langle p' \underset{\sim}{\Omega}, \sigma'' | E', \lambda' \rangle (-2e^{i\eta'} \sin\eta') \langle E', \lambda' | \underset{\sim}{p}', \sigma' \rangle \right|^2 \\
&= 4(2\pi/p')^{N-1} \left| \sum_{\lambda'} e^{i\eta'} \sin\eta' \, \mathcal{Y}_{\lambda'}(E', \underset{\sim}{\Omega}, \sigma'') \mathcal{Y}_{\lambda'}{}^{*}(E', \underset{\sim}{\Omega}', \sigma') \right|^2 .
\end{aligned} \tag{8.46}$$

The total cross section for $N \geqslant 2$ can be obtained either directly from (8.30) or by integration of (8.46) with use of (8.43). The result is

$$\sigma(\underset{\sim}{p}', \sigma') = 4(2\pi/p')^{N-1} \sum_{\lambda'} \left| \mathcal{Y}_{\lambda'}(E', \underset{\sim}{\Omega}', \sigma') \right|^2 \sin^2 \eta' . \tag{8.47}$$

<u>The case of spherical symmetry.</u>

In practical cases the functions $\mathcal{Y}_{\lambda'}$ are often completely determined by the symmetry properties of the system H. Thus, for example, if the perturbation H_1 is a potential $V(r)$ which is a function only of the absolute value of the position vector $\underset{\sim}{r}$ of the particle, the $\mathcal{Y}_{\lambda'}$ are the N-dimensional spherical harmonics and are therefore independent of the energy and of the labels σ'. In this case the significance of the operator η will be seen by passing to the coordinate representation.

Use of (8.15) and the equation

$$\langle \underset{\sim}{r} | \underset{\sim}{p}' \rangle = (d^N \underset{\sim}{r}/L^N)^{\frac{1}{2}} e^{i \underset{\sim}{p}' \cdot \underset{\sim}{r}} \tag{8.48}$$

gives

$$\begin{aligned} \langle \underset{\sim}{r} | E', \lambda' \rangle &= \sum{}'' \langle \underset{\sim}{r} | \underset{\sim}{p}'' \rangle \langle \underset{\sim}{p}'' | E', \lambda' \rangle \\ &= (d^N \underset{\sim}{r})^{\frac{1}{2}} (2\pi)^{-\frac{1}{2}(N-1)} (p'^{N-1}/v'T')^{\frac{1}{2}} \int e^{i p' r \underset{\sim}{\Omega}'' \cdot \underset{\sim}{\Omega}} \mathcal{Y}_{\lambda'}(\underset{\sim}{\Omega}'') d^{N-1} \underset{\sim}{\Omega}'' . \end{aligned} \tag{8.49}$$

Here the labels σ' have been dropped.

<u>Phase shifts in one dimension.</u>

In the one-dimensional problem λ' is simply a parity label, the functions $\mathcal{Y}_{\lambda'}$ being given by

$$\mathcal{Y}_{\lambda'}(\pm 1) = (\pm 1)^{\lambda'}/\sqrt{2} \quad ; \qquad \lambda' = 0, 1 \quad ; \tag{8.50}$$

yielding

$$\langle \underset{\sim}{r} | E', \lambda' \rangle = (d^1\underset{\sim}{r}/v'T')^{\frac{1}{2}} \left[e^{i\,p'r} + (-1)^{\lambda'} e^{-i\,p'r} \right] \mathcal{Y}_{\lambda'}(\underset{\sim}{\Omega}) . \tag{8.51}$$

Now, in section 4 we discussed the asymptotic behavior of the scattering wave functions in terms of a set of vectors $|\mathrm{ret}'\rangle$, $|\mathrm{adv}'\rangle$ and their differences $|\mathrm{rad}'\rangle$. Comparison of Eqs. (4.24) and (7.44) shows that

$$|\mathrm{rad}'\rangle = -i\,\underset{\sim}{R}_+ |\underset{\sim}{p}'\rangle \tag{8.52}$$

$$= 2\,i\,e^{i\eta} \sin\eta |\underset{\sim}{p}'\rangle . \tag{8.53}$$

Taking the coordinate representation of Eq. (8.53), using Eqs. (8.42) and (8.51), and remembering that the vectors $|\mathrm{ret}'\rangle$ and $|\mathrm{adv}'\rangle$ are made unique by the boundary conditions (4.12, 14) and the requirement that they satisfy the Schrödinger equation of the system H_o everywhere except at the origin, one easily makes the identification

$$\langle \underset{\sim}{r} | \mathrm{ret}' \rangle = 2i\,(d^1\underset{\sim}{r}/L)^{\frac{1}{2}} \sum_{\lambda'} e^{i(p'r+\eta')} \sin\eta'\, \mathcal{Y}_{\lambda'}(\underset{\sim}{\Omega})\, \mathcal{Y}_{\lambda'}^{*}(\underset{\sim}{\Omega}') . \tag{8.54}$$

The eigenvector $|\underset{\sim}{p}_+'\rangle$ of H therefore has the asymptotic behavior

$$\langle \underset{\sim}{r} | \underset{\sim}{p}_+' \rangle \sim \langle \underset{\sim}{r} | \underset{\sim}{p}' \rangle + \langle \underset{\sim}{r} | \mathrm{ret}' \rangle$$

$$= \tfrac{1}{2}(d^1\underset{\sim}{r}/L)^{\frac{1}{2}} \sum_{\lambda'} e^{i\eta'} \left[e^{i(p'r+\eta')} + (-1)^{\lambda'} e^{-i(p'r+\eta')} \right] (\underset{\sim}{\Omega}\cdot\underset{\sim}{\Omega}')^{\lambda'} , \tag{8.55}$$

which shows explicitly the interpretation of the eigenvalues of η as phase shifts induced by the perturbation H_1 in the so-called "partial waves" out of which the plane wave $\langle \underset{\sim}{r} | \underset{\sim}{p}' \rangle$ may be constructed.

The transmission and reflection coefficients are readily expressed in terms of the phase shifts:

$$R(\underset{\sim}{p}') = \sigma(-\underset{\sim}{\Omega}' | \underset{\sim}{p}') = \left| \sum_{\lambda'} (-1)^{\lambda'} e^{i\eta'} \sin\eta' \right|^2$$

$$= \sin^2 \left[\eta_0(E') - \eta_1(E') \right] , \tag{8.56}$$

$$T(\underset{\sim}{p}') = \cos^2 \left[\eta_0(E') - \eta_1(E') \right] , \tag{8.57}$$

where $\eta' = \eta_{0,1}(E')$ for $\lambda' = 0, 1$.

In practice the phase shifts can be computed either by numerical integration of a radial wave function or by solving an integral equation. The pertinent relations in the latter case are determined by Eqs. (7.52) and (7.59) together with the conveniently introduced functions

$$K_{\lambda'}(p'' | p') = \tfrac{1}{2}(v'' T'' v' T')^{\frac{1}{2}} \langle E'', \lambda' | K(E') | E', \lambda' \rangle , \tag{8.58}$$

$$V_{\lambda'}(p'' | p') = \tfrac{1}{2}(v'' T'' v' T')^{\frac{1}{2}} \langle E'', \lambda' | H_1 | E', \lambda' \rangle$$

$$= \begin{cases} 2\int_0^\infty \cos p''r \, V(r) \cos p'r \, dr , & \lambda' = 0 , \\ 2\int_0^\infty \sin p''r \, V(r) \sin p'r \, dr , & \lambda' = 1 . \end{cases} \tag{8.59}$$

Use of the formal relation $\sum_{E'''} = \int (T'''/2\pi) dE'''$ puts Eq. (7.52) in the form

$$K_{\lambda'}(p'' | p') = V_{\lambda'}(p'' | p') + \frac{1}{\pi} \mathcal{P} \int_0^\infty \frac{V_{\lambda'}(p'' | p''')}{E' - E'''} K_{\lambda'}(p''' | p') dp''' . \tag{8.60}$$

The solution of this integral equation yields the phase shifts in the form

$$\tan \eta' = -v'^{-1} K_{\lambda'}(p' \mid p') . \tag{8.61}$$

Two dimensions.

The two-dimensional scattering problem has considerable interest in acoustics and optics, but is of no importance in quantum mechanics and will not be discussed here.

Three dimensions.

In the case of three dimensions the $\mathcal{Y}_{\lambda'}$ become the ordinary spherical harmonics

$$\mathcal{Y}_{\lambda'}(\underset{\sim}{\Omega}) \rightarrow Y_l^m(\underset{\sim}{\Omega}) ; \qquad m = -l, \ldots l ; \qquad l = 0, 1, 2, \ldots ; \tag{8.62}$$

which, when substituted into (8.49), give

$$\langle \underset{\sim}{r} \mid E', l, m \rangle = (d^3\underset{\sim}{r})^{\frac{1}{2}} (2\pi)^{-1} (p'^2/v'T')^{\frac{1}{2}} 4\pi i^l j_l(p'r) Y_l^m(\underset{\sim}{\Omega}) \tag{8.63}$$

where the j_l are the spherical Bessel functions:

$$j_l(p'r) = (\pi/2p'r)^{\frac{1}{2}} J_{l+\frac{1}{2}}(p'r) \tag{8.64}$$

$$\sim (-i)^l (2ip'r)^{-1} \left[e^{ip'r} - (-1)^l e^{-ip'r} \right] . \tag{8.65}$$

The eigenvalues of η are independent of the label m and may be written

$$\eta' = \eta_l(E') . \tag{8.66}$$

Therefore the theorem

$$\sum_m Y_l^m(\underset{\sim}{\Omega}) Y_l^{m*}(\underset{\sim}{\Omega}') = (4\pi)^{-1}(2l+1) P_l(\underset{\sim}{\Omega} \cdot \underset{\sim}{\Omega}') \tag{8.67}$$

may be used to put the "retarded wave" in the form

$$\langle \underset{\sim}{r} | \text{ret}' \rangle = 2i(d^3\underset{\sim}{r}/L^3)^{\frac{1}{2}} \sum_l \tfrac{1}{2}\, i^l (2l+1) e^{i\eta_l} \sin\eta_l \, h_l^{(1)}(p'r)\, P_l(\underset{\sim}{\Omega}\cdot\underset{\sim}{\Omega}'). \tag{8.68}$$

Here the P_l are the Legendre polynomials, and the $h_l^{(1)}$ are the spherical Hankel functions* satisfying

$$h_l^{(1)}(p'r) \sim (-i)^l \, (i\, p'r)^{-1} \, e^{i\, p'r} , \tag{8.69}$$

$$j_l = \tfrac{1}{2}(h_l^{(1)} + h_l^{(1)*}) . \tag{8.70}$$

The eigenvector $| \underset{\sim}{p}_+' \rangle$ now has the asymptotic form

$$\langle \underset{\sim}{r} | \underset{\sim}{p}_+' \rangle$$
$$\sim (d^3\underset{\sim}{r}/L^3)^{\frac{1}{2}} \sum_l (2l+1)(2ip'r)^{-1} e^{i\eta_l} \left[e^{i(p'r+\eta_l)} - (-1)^l e^{-i(p'r+\eta_l)} \right]$$
$$\times P_l(\underset{\sim}{\Omega}\cdot\underset{\sim}{\Omega}') , \tag{8.71}$$

showing again the interpretation of the η_l as phase shifts.

The angular and total cross sections have the familiar forms

$$\sigma(\underset{\sim}{\Omega} | \underset{\sim}{p}') = p'^{-2} \left| \sum_l (2l+1) e^{i\eta_l} \sin\eta_l \, P_l(\underset{\sim}{\Omega}\cdot\underset{\sim}{\Omega}') \right|^2 \tag{8.72}$$

$$\sigma(\underset{\sim}{p}') = 4\pi\, p'^{-2} \sum_l (2l+1) \sin^2\eta_l(E') . \tag{8.73}$$

The tangent of the phase shift may be computed from

$$\tan\eta_l(E') = -v'^{-1} K_l(p' | p') \tag{8.74}$$

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* For definitions see, for example, L. I. Schiff, Quantum Mechanics (New York, McGraw-Hill, 1949) p.77.

where

$$K_l(p''|p') = V_l(p''|p') + \frac{1}{\pi} \mathcal{P} \int_0^\infty \frac{V_l(p''|p''')}{E' - E'''} K_l(p'''|p')\, dp''' \tag{8.75}$$

with

$$V_l(p''|p') = 2\, p''\, p' \int_0^\infty j_l(p''r)\, V(r)\, j_l(p'r)\, r^2\, dr\ . \tag{8.76}$$

<u>The reverse scattering theorem.</u>

Even when the scattering force is not spherically symmetric certain relations continue to exist, which may be quickly demonstrated with the aid of the operator formalism. For instance

$$\sigma(\underset{\sim}{\Omega}''|\underset{\sim}{p}') = \sigma(-\underset{\sim}{\Omega}'|-\underset{\sim}{p}''), \qquad E'' = E' \quad , \tag{8.77}$$

regardless of the spatial dependence of the force, provided that if the force has any momentum dependence, this dependence be only on the absolute value of the momentum. H_1 then has the general form

$$H_1 = \sum_i \left[f_i(p)\, V_i(\underset{\sim}{r}) + V_i(\underset{\sim}{r})\, f_i(p)\right] , \tag{8.78}$$

and its matrix elements are

$$\left\langle \underset{\sim}{p}'' \middle| H_1 \middle| \underset{\sim}{p}' \right\rangle = \sum_i \left[f_i(p'') + f_i(p')\right] v_i(\underset{\sim}{p}'' - \underset{\sim}{p}') \tag{8.79}$$

where

$$v_i(\underset{\sim}{p}') = L^{-N} \int e^{-i\, \underset{\sim}{p}' \cdot \underset{\sim}{r}}\, V_i(\underset{\sim}{r})\, d^N\underset{\sim}{r}\ . \tag{8.80}$$

Evidently

$$\left\langle -\underset{\sim}{p}'' \middle| H_1 \middle| -\underset{\sim}{p}' \right\rangle = \left\langle \underset{\sim}{p}' \middle| H_1 \middle| \underset{\sim}{p}'' \right\rangle \quad , \tag{8.81}$$

and it is easily verified, by expanding Eq. (7.2) and remembering that E' depends only on p', that

$$\left\langle -\underset{\sim}{p}'' \middle| R_{\pm} \middle| -\underset{\sim}{p}' \right\rangle = \left\langle \underset{\sim}{p}' \middle| R_{\pm} \middle| \underset{\sim}{p}'' \right\rangle, \qquad E'' = E' , \tag{8.82}$$

which leads, via (8.19), to (8.77). Thus <u>the cross section for scattering along a given angular path is equal to that for the reverse path</u>. In the one-dimensional case this reduces to the well known theorem that the transmission (or reflection) coefficients from the right and left are identical regardless of the shape of the potential.

<u>The one-dimensional delta-function potential.</u> [21,48]

An example which illustrates many of the features of perturbation theory considered in this article, but which is nevertheless so simple that it is completely solvable in all respects, is afforded by the system $H = H_0 + H_1$ with

$$H_0 = \tfrac{1}{2} p^2 , \qquad H_1 = - g\,\delta(\underset{\sim}{r}), \tag{8.83}$$

where $\underset{\sim}{r}$ is a one-dimensional coordinate. Use of the relations

$$dr/d\underset{\sim}{r} = \underset{\sim}{r}/r , \qquad d^2r/d\underset{\sim}{r}^2 = 2\,\delta(\underset{\sim}{r}) , \tag{8.84}$$

leads readily to the coordinate representation of the eigenvectors of H:

$$\left\langle \underset{\sim}{r} \middle| \underset{\sim}{p}_{\pm}' \right\rangle = (L^{-1} d^1\underset{\sim}{r})^{\frac{1}{2}} \left[e^{i\,\underset{\sim}{p}'\cdot\underset{\sim}{r}} - g(g \pm i\,p')^{-1} e^{\pm i\,p'r} \right], \tag{8.85}$$

with

$$E' = \tfrac{1}{2} p'^2 , \qquad v' = p' . \tag{8.86}$$

If $g > 0$ there is also one bound state $|J'\rangle$ given by

$$\langle \underset{\sim}{r} | J' \rangle = (g\, d^1\underset{\sim}{r})^{\frac{1}{2}}\, e^{-gr} , \tag{8.87}$$

with

$$E' = -\tfrac{1}{2} g^2 . \tag{8.88}$$

The orthonormality of the vectors $|\underset{\sim}{p}_\pm'\rangle$, $|J'\rangle$ is readily demonstrated from Eqs. (8.85), (8.87). Of interest is also the demonstration of their completeness. After a little reduction one easily obtains

$$\begin{aligned}
&\sum{}' \langle \underset{\sim}{r}''' | \underset{\sim}{p}_\pm' \rangle \langle \underset{\sim}{p}_\pm' | \underset{\sim}{r}'' \rangle \\
&= d^1\underset{\sim}{r} \left[\delta(\underset{\sim}{r}''' - \underset{\sim}{r}'') - (2\pi)^{-1} \int_{-\infty}^{\infty} g(g \pm i\, p')^{-1}\, e^{\pm i\, p'(r'' + r''')}\, dp' \right] \\
&= \delta_{\underset{\sim}{r}'''\underset{\sim}{r}''} - \theta_+(g) \langle \underset{\sim}{r}''' | J' \rangle \langle J' | \underset{\sim}{r}'' \rangle ,
\end{aligned} \tag{8.89}$$

showing that the vectors $|\underset{\sim}{p}_\pm'\rangle$ are complete when $g < 0$ and incomplete by just the amount of the bound state vector $|J'\rangle$ when $g > 0$.

The S-matrix can be determined by inspection from (8.85). Evidently

$$\langle \underset{\sim}{r} | \mathrm{ret}' \rangle = -(L^{-1}\, d^1\underset{\sim}{r})^{\frac{1}{2}}\, g(g + i\, p')^{-1}\, e^{i\, p' r} , \tag{8.90}$$

$$\langle \underset{\sim}{r} | \mathrm{adv}' \rangle = (L^{-1}\, d^1\underset{\sim}{r})^{\frac{1}{2}}\, g(g + i\, p')^{-1}\, e^{-i\, p' r} , \tag{8.91}$$

$$\langle \underset{\sim}{r} | \mathrm{rad}' \rangle = -2(L^{-1}\, d^1 r)^{\frac{1}{2}}\, g(g + i\, p')^{-1} \cos p' r , \tag{8.92}$$

so that

$$\begin{aligned}
\langle \underset{\sim}{p}'' | S | \underset{\sim}{p}' \rangle &= \delta_{\underset{\sim}{p}''\underset{\sim}{p}'} + \langle \underset{\sim}{p}'' | \mathrm{rad}' \rangle \\
&= \delta_{\underset{\sim}{p}''\underset{\sim}{p}'} - g(g + i\, p')^{-1} (\delta_{\underset{\sim}{p}''\underset{\sim}{p}'} + \delta_{-\underset{\sim}{p}''\underset{\sim}{p}'}) .
\end{aligned} \tag{8.93}$$

The unitarity of the S-matrix may be verified directly from (8.93).

The S-matrix may readily be diagonalized with the aid of (8.42) and (8.50), the result giving for the phase shifts

$$\eta_0(E') = \tan^{-1}(g/p') , \tag{8.94}$$

$$\eta_1(E') = 0 , \tag{8.95}$$

and for the reactance matrix

$$\left\langle \underset{\sim}{p}'' \middle| \underset{\sim}{K} \middle| \underset{\sim}{p}' \right\rangle = -(g/p')(\delta_{\underset{\sim}{p}''\underset{\sim}{p}'} + \delta_{-\underset{\sim}{p}''\underset{\sim}{p}'}) . \tag{8.96}$$

The transmission and reflection coefficients are

$$T(\underset{\sim}{p}') = p'^2/(g^2 + p'^2) , \tag{8.97}$$

$$R(\underset{\sim}{p}') = g^2/(g^2 + p'^2) . \tag{8.98}$$

Of interest also are the momentum representations of the eigenvectors $\left| \underset{\sim}{p}_\pm' \right\rangle$ and $\left| J' \right\rangle$, which can be obtained by carrying out the unitary transformation (8.48) on Eqs. (8.85) and (8.87):

$$\left\langle \underset{\sim}{p}'' \middle| \underset{\sim}{p}_\pm' \right\rangle = \delta_{\underset{\sim}{p}''\underset{\sim}{p}'} - i\, L^{-1}\, g(g \pm i\, p')^{-1} \left(\frac{1}{\underset{\sim}{p}'' \pm p' + i\epsilon'} - \frac{1}{\underset{\sim}{p}'' \mp p' - i\epsilon'} \right)$$

$$= \delta_{\underset{\sim}{p}''\underset{\sim}{p}'} \mp i\, L^{-1} \frac{1}{E' - E'' \pm i\epsilon} \frac{gp'}{g \pm i\, p'} , \tag{8.99}$$

$$\left\langle \underset{\sim}{p}'' \middle| J' \right\rangle = (g\, L^{-1})^{\frac{1}{2}}\ 2g/(g^2 + p''^2) . \tag{8.100}$$

An infinitesimal damping coefficient, $\epsilon' = \epsilon/p'$, has been introduced in the integrals which evaluate (8.99).

Eqs. (7.8) and (8.99) allow one to infer

$$\left\langle \underset{\sim}{p}'' \middle| R_{\pm}(E') \middle| \underset{\sim}{p}' \right\rangle = \mp i\, L^{-1}\, gp'/(g \pm i\, p') \,. \tag{8.101}$$

This result may be verified directly by expanding (7.2). One needs for this purpose the momentum matrix elements of H_1,

$$\left\langle \underset{\sim}{p}'' \middle| H_1 \middle| \underset{\sim}{p}' \right\rangle = -\, g\, L^{-1} \,, \tag{8.102}$$

which give, with the aid of the integral

$$\int_{-\infty}^{\infty} (p'^2 - p^2 \pm i\alpha)^{-1}\, dp = \mp \pi\, i (p'^2 \pm i\alpha)^{-\frac{1}{2}} \,, \qquad \alpha > 0 \,, \tag{8.103}$$

the series

$$\left\langle \underset{\sim}{p}'' \middle| R_{\pm}(E') \middle| \underset{\sim}{p}' \right\rangle = -\, g\, L^{-1} \sum_{n=0}^{\infty} (\pm i\, g/p')^n \,. \tag{8.104}$$

in the limit $\epsilon \to 0$. Expansion (8.104) converges to (8.101) when $p' > g$.

In a similar manner the reactance matrix (8.96) may be obtained by expanding (7.51). In this case only the first term of the series is non-vanishing since

$$\mathcal{P} \int_{-\infty}^{\infty} (p'^2 - p^2)^{-1}\, dp = 0 \,. \tag{8.105}$$

Therefore

$$\left\langle \underset{\sim}{p}'' \middle| \underset{\sim}{K} \middle| \underset{\sim}{p}' \right\rangle = -\, 2\pi\, g\, L^{-1} \delta\, (E'' - E') \,, \tag{8.106}$$

which is equivalent to (8.96) in virtue of the fact that

$$\begin{aligned} \delta_{\underset{\sim}{p}''\underset{\sim}{p}'} + \delta_{-\underset{\sim}{p}''\underset{\sim}{p}'} = \delta_{E''E'} &= (2\pi/T')\, \delta(E'' - E') \\ &= (2\pi p'/L)\, \delta\, (E'' - E') \,, \end{aligned} \tag{8.107}$$

where (8.86) and the relation $L = v'T'$ have been used.

9. BOUND STATE PERTURBATION THEORY

The use of contour integration

The theory of perturbations for bound systems differs in many respects from scattering theory because of the discreteness of the bound-state energy levels. This discreteness enables one to use a number of analytical devices which are unavailable in the continuum case. For example, the singularities of the operators $G_{0\pm}(E)$, $G_{\pm}(E)$ are separate simple poles in the complex E-plane, and closed contours may be drawn which isolate zero, one, or a small finite number of them. We shall make use of integrations over such contours, following a method due to Kato. [56]

In performing these integrations it will be noted that the presence of the imaginary terms $\pm i\epsilon$ is immaterial, and therefore we shall introduce at once the operators

$$G_0(E) = \frac{1}{E - H_0}, \tag{9.1}$$

$$G(E) = \frac{1}{E - H} = G_0(E)\left[1 - H_1 G_0(E)\right]^{-1}. \tag{9.2}$$

Let each singularity H_0' of $G_0(E)$ be surrounded by a separate contour C' in such a way that the regions enclosed by the contours do not overlap one another. Then

$$(2\pi i)^{-1} \oint_{C'} G_0(E)\, dE = (2\pi i)^{-1} \oint_{C'} \sum{}'' \left|J_0''\right\rangle (E - H_0'')^{-1} \left\langle J_0''\right| dE$$

$$= P_0^{(')} \tag{9.3}$$

where $P_0^{(')}$ is the projection operator on the eigenstates of H_0 which have the eigenvalue H_0':

$$P_o^{(')} = \sum{}'' \left|J_o''\right\rangle \delta(H_o', H_o'') \left\langle J_o''\right| \quad . \tag{9.4}$$

The eigenvectors and eigenvalues of H will generally depend in a continuous fashion on the coupling constant g of (5.19) in the neighborhood of $g = 0$.* The projection operator $P_o^{(')}$ will therefore pass continuously into an idempotent operator $\mathfrak{P}^{(')}$ as g departs from zero. In order to account for a possible level splitting in case the original level H_o' is degenerate, one may write

$$\mathfrak{P}^{(')} = \sum{}'' \delta(H_o', H_o'') \, P^{('')} \tag{9.5}$$

where $P^{('')}$ is the projection operator on the eigenstates of H which have the eigenvalue $H'' = E''$:

$$P^{('')} = \sum{}''' \left|J'''\right\rangle \delta_{E''E'''} \left\langle J'''\right| \quad , \tag{9.6}$$

and where the summation in Eq. (9.5) counts each $P^{('')}$ only once. Here our notation assumes the existence of a one-to-one correspondence between the eigenvectors of H and an appropriate set of eigenvectors of H_o:

$$\left|J_o''\right\rangle, H_o'' \longleftrightarrow \left|J''\right\rangle, E'' \quad . \tag{9.7}$$

It is not necessary to know here how such a correspondence will finally be set up, because for the time being we may work directly with the operators $P_o^{(')}$, $\mathfrak{P}^{(')}$. It is only necessary to know that the subspaces defined by $P_o^{(')}$ and $\mathfrak{P}^{(')}$ have the same dimensionality.

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* This is true even for field theories as long as the high energy cut-off is kept finite. The cut-off may be allowed to become infinite only after all formal calculations have been carried out.

$$d' = \mathrm{Tr}\, P_o^{(')} = \mathrm{Tr}\, \mathcal{P}^{(')} = \sum{}'' \delta(H_o', H_o'')\, \mathrm{Tr}\, P^{('')} , \tag{9.8}$$

measuring the degree of degeneracy of the level H_o'.

If g is small enough so that the levels E'' into which the levels H_o' split (or shift) all remain inside their respective contours C' then

$$\mathcal{P}^{(')} = (2\pi i)^{-1} \oint_{C'} G(E)\, dE . \tag{9.9}$$

It is useful also to define the related operator

$$\Delta^{(')} = (2\pi i)^{-1} \oint_{C'} (E - H_o')\, G(E)\, dE . \tag{9.10}$$

In virtue of the identity

$$(E - H_o')\, G(E) = 1 + (H - H_o')\, G(E) \tag{9.11}$$

it is evident that

$$\Delta^{(')} = (H - H_o')\, \mathcal{P}^{(')} = \sum{}'' \delta(H_o', H_o'')\, \Delta E''\, P^{('')} \tag{9.12}$$

where the $\Delta E''$ are the level shifts. The operators $\mathcal{P}^{(')}$ and $\Delta^{(')}$ play the basic roles in bound state perturbation theory.

Series expansions.

For practical computations it is necessary to have series expansions of the operators $\mathcal{P}^{(')}$ and $\Delta^{(')}$. Evidently, from (9.2),

$$\mathcal{P}^{(')} = \sum_{n=0}^{\infty} P_n^{(')} , \tag{9.13a}$$

$$\Delta^{(')} = \sum_{n=1}^{\infty} \Delta_n^{(')} , \tag{9.14a}$$

where

$$P_n^{(\prime)} = (2\pi i)^{-1} \oint_{C'} G_0(E) \left[H_1 G_0(E) \right]^n dE \ , \tag{9.13b}$$

$$\Delta_n^{(\prime)} = (2\pi i)^{-1} \oint_{C'} (E - H_o') \, G_0(E) \left[H_1 G_0(E) \right]^n dE \ . \tag{9.14b}$$

The integrals (9.13b) and (9.14b) may be evaluated by separating out the singularity of $G_0(E)$ at H_o', writing

$$G_0(E) = \frac{P_0^{(\prime)}}{E - H_o'} + \frac{1 - P_0^{(\prime)}}{E - H_o'}$$

$$= \frac{P_0^{(\prime)}}{E - H_o'} + \frac{1 - P_0^{(\prime)}}{H_o' - H_o} \left(1 + \frac{E - H_o'}{H_o' - H_o} \right)^{-1} \tag{9.15}$$

and then expanding the bracketed inverse by the rule

$$(1 - x)^{-1} = 1 + x + \ldots + x^{n-1} + x^n (1 - x)^{-1} \ . \tag{9.16}$$

One gets

$$P_n^{(\prime)} = - \sum_{\substack{k_i \geq 0 \\ k_1 + \ldots + k_{n+1} = n}} \mathcal{G}_{k_1}^{(\prime)} H_1 \, \mathcal{G}_{k_2}^{(\prime)} H_1 \ldots H_1 \, \mathcal{G}_{k_{n+1}}^{(\prime)} \ , \tag{9.13c}$$

$$\Delta_n^{(\prime)} = \sum_{\substack{k_i \geq 0 \\ k_1 + \ldots + k_{n+1} = n - 1}} \mathcal{G}_{k_1}^{(\prime)} H_1 \mathcal{G}_{k_2}^{(\prime)} H_1 \ldots H_1 \mathcal{G}_{k_{n+1}}^{(\prime)} \ , \tag{9.14c}$$

where

$$\mathcal{G}_0^{(\prime)} = - P_0^{(\prime)} \ , \tag{9.17}$$

$$\mathcal{G}_k^{(\prime)} = \frac{1 - P_0^{(\prime)}}{(H_o' - H_o)^k} \ , \qquad k \geq 1 \ . \tag{9.18}$$

It may be verified by direct computation, and use of $P_0^{(\prime)2} = P_0^{(\prime)}$, that expansions (9.13, 14) satisfy the identities

$$\mathfrak{P}^{(\prime)2} = \mathfrak{P}^{(\prime)} , \tag{9.19}$$

$$\mathfrak{P}^{(\prime)} \Delta^{(\prime)} = \Delta^{(\prime)} \mathfrak{P}^{(\prime)} = \Delta^{(\prime)} . \tag{9.20}$$

On the other hand, the further necessary identities

$$\mathfrak{P}^{(\prime)} \mathfrak{P}^{(\prime\prime)} = 0 , \qquad H_0^{\prime} \neq H_0^{\prime\prime} \tag{9.21}$$

$$\mathfrak{P}^{(\prime)} \Delta^{(\prime\prime)} = \Delta^{(\prime\prime)} \mathfrak{P}^{(\prime)} = 0 , \qquad H_0^{\prime} \neq H_0^{\prime\prime} , \tag{9.22}$$

cannot be derived from the expansions. They will, however, be satisfied by the expansions as long as the smallness of g keeps the perturbed levels within their respective contours.

<u>Computation of the $|J^{\prime}\rangle$ and $\Delta E^{\prime}$.</u>

The level shifts $\Delta E^{\prime}$ are determined by diagonalizing the operators $\Delta^{(\prime)}$ in their respective subspaces $\mathfrak{P}^{(\prime)}$. In order to do this it is first necessary to construct an orthonormal basis in each subspace. This is most easily accomplished by diagonalizing the Hermitian operators $P_0^{(\prime)} \mathfrak{P}^{(\prime)} P_0^{(\prime)}$. With respect to an eigenbasis of H_0 these operators are generally finite matrices, and hence their diagonalization is usually a manageable mathematical problem. In practice one computes these matrices approximately by carrying out expansion (9.13) up to a certain order in g, and then one solves the corresponding secular determinant by any one of a variety of techniques. Since these techniques are not of particular interest in this article we shall simply assume that the diagonalization has already been carried out and write

$$\delta(H_o'', H_o')\langle \mathcal{J}_o'' | \mathcal{P}^{(1)} | \mathcal{J}_o' \rangle = \mathcal{Z}' \delta(\mathcal{J}_o'', \mathcal{J}_o'), \tag{9.23}$$

the $|\mathcal{J}_o'\rangle$ being appropriate eigenvectors of H_o which effect the diagonalization, and the $\mathcal{Z}'$ being the corresponding eigenvalues. An orthonormal basis which is congruent to the subspaces $\mathcal{P}^{(1)}$ is now provided by the vectors

$$|\mathcal{J}'\rangle = \mathcal{Z}'^{-\frac{1}{2}} \mathcal{P}^{(1)} |\mathcal{J}_o'\rangle . \tag{9.24}$$

The remaining task is the diagonalization of the matrices

$$\langle \mathcal{J}'' | \Delta^{(1)} | \mathcal{J}' \rangle = \delta(H_o'', H_o')(\mathcal{Z}''\mathcal{Z}')^{-\frac{1}{2}} \langle \mathcal{J}_o'' | \Delta^{(1)} | \mathcal{J}_o' \rangle . \tag{9.25}$$

These are again finite Hermitian matrices, and the same standard mathematical techniques as before can be used. The eigenvectors $|J'\rangle$ of H are defined by the unitary transformation $\langle \mathcal{J}'' | J' \rangle$ which performs the diagonalization:

$$\langle J'' | \Delta^{(1)} | J' \rangle = \delta_{J''J'} \Delta E' . \tag{9.26}$$

If, in the approximate evaluation of $\Delta^{(1)}$, expansion (9.14) is carried out to a given order in g, this order of accuracy will be reflected in the computed level shifts $\Delta E'$ provided only that the accompanying expansion of $\mathcal{P}^{(1)}$ is carried out to an order of accuracy less by one.

Once the eigenvectors $|J'\rangle$ of H have been determined the one-to-one correspondence (9.7) with the eigenvectors of H_o can be set up by defining

$$|J_o'\rangle = \lim_{g \to 0} |J'\rangle . \tag{9.27}$$

However, in the above computation of the $|J'\rangle$ and $\Delta E'$ the vectors $|J_0'\rangle$ never come into the picture. It is to be noted that the vectors $|\mathcal{J}_0'\rangle$ are generally <u>not</u> identical with the $|J_0'\rangle$.

<u>Progressive removal of degeneracy.</u>

If the eigenvalues of the operator $P_0^{(')}\Delta_1^{(')}P_0^{(')} = P_0^{(')}H_1P_0^{(')}$ are all distinct in the subspace $P_0^{(')}$ then it is easy to see that the $|J_0''\rangle$ with $H_0'' = H_0'$ are simply the eigenvectors of H_0 which diagonalize this operator. To lowest order in g the level shifts are the eigenvalues in question. If these eigenvalues are not all distinct the $|J_0'\rangle$ are not completely determined by this prescription, and a more complicated study is necessary, involving the operators $P_1^{(')}$ and $\Delta_2^{(')}$. However, the observation serves as initial motivation for a procedure of progressive removal of any degeneracy which may happen to be present in the system H_0 and the development of a perturbation theory in which the vectors $|J_0'\rangle$ play a more direct role.

Instead of expanding the operators $\mathcal{P}^{(')}$, $\Delta^{(')}$ and then diagonalizing, one begins by simply diagonalizing $P_0^{(')}\Delta_1^{(')}P_0^{(')}$ and then making the replacements

$$\begin{aligned} H_0 &\rightarrow H_0 + \sum{}' P_0^{(')}\Delta_1^{(')}P_0^{(')} \\ H_1 &\rightarrow H_1 - \sum{}' P_0^{(')}\Delta_1^{(')}P_0^{(')} \end{aligned} \tag{9.28a}$$

(Here the summation $\sum'$ counts each distinct eigenvalue of H_0 only once.) If some of the $P_0^{(')}\Delta_1^{(')}P_0^{(')}$ have eigenvalues which are not all identical (in their respective subspaces) then the replacement (9.28a) removes some of the degeneracy. If the system H_0 possesses any

remaining degeneracy this degeneracy will not be removed to first order by the new perturbation H_1. To carry out a further removal of the degeneracy it is necessary to diagonalize the operators $P_0^{(')} \Delta_2^{(')} P_0^{(')}$ (defined with respect to the new operators H_0, H_1) and make the replacement

$$H_0 \rightarrow H_0 + \sum{}' P_0^{(')} \Delta_2^{(')} P_0^{(')}$$

$$H_1 \rightarrow H_1 - \sum{}' P_0^{(')} \Delta_2^{(')} P_0^{(')} . \tag{9.28b}$$

If the degneracy is still not completely removed one may go on, this time replacing $\Delta_2^{(')}$ by $\Delta_3^{(')}$, and so on. Eventually, either all the degeneracy will be removed or else a degeneracy will remain which is nonremovable.* The origin of nonremovable degeneracy lies in special symmetry properties possessed by the perturbation H_1, which leave it diagonal in some of the labels J_0' with the values of its nonvanishing matrix elements depending only on the remaining labels. The former labels simply enumerate the states within the various degenerate levels. Nonremovable degeneracy is generally very easy to spot.

When removable degeneracy is absent any set of eigenvectors of H_0 may be used in setting up the one-to-one correspondence (9.7). The operators $P_0^{(')} \mathcal{B}^{(')} P_0^{(')}$ are then simply multiples of the operators $P_0^{(')}$, the factors of proportionality being the normalization constants Z' of Eq. (6.8):

$$P_0^{(')} \mathcal{B}^{(')} P_0^{(')} = Z' P_0^{(')} . \tag{9.29}$$

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* All degeneracy could, of course, be removed at the very beginning by an arbitrary redefinition of H_0. The present systematic method, however, generally insures the most rapid convergence of the perturbation calculations remaining after the removal.

The eigenvectors of H are given by

$$\left| J' \right\rangle = z'^{-\frac{1}{2}} \mathcal{P}^{(')} \left| J_o' \right\rangle . \tag{9.30}$$

Furthermore the operators $\Delta^{(')}$ are simple multiples of the operators $\mathcal{P}^{(')}$,

$$\Delta^{(')} = \Delta E' \mathcal{P}^{(')} , \tag{9.31}$$

so that the level shifts may be computed from the simple formula

$$\Delta E' = d'^{-1} \operatorname{Tr} \mathcal{P}^{(')} . \tag{9.32}$$

<u>The Rayleigh-Schrödinger perturbation formula.</u>

If expansion (9.14) is inserted into Eq. (9.32) then, owing to the cyclic invariance of the trace, the following equation results:

$$\Delta E' = d'^{-1} \sum_{n=1}^{\infty} \sum_{k_1 + \cdots + k_n = n-1}^{k_i \geq 0} (k_n - 1) \operatorname{Tr} H_1 \mathcal{G}_{k_1}^{(')} \cdots H_1 \mathcal{G}_{k_n}^{(')} . \tag{9.33}$$

This equation may be further simplified through the observation that the factors occurring in the summand can be cyclically rearranged in n different orders, each giving the same trace. One of these orders may be chosen as standard. If only the standard order is allowed in the summation then the numerical factor $(k_n - 1)$ in front of the trace must be replaced by $\sum_i (k_i - 1) = -1$. Suppose the standard order is one in which $k_n = 0$. This does not uniquely specify the standard order, for there are N_k other orders which meet this specification, N_k being the number of remaining indices k_i, $i < n$, which are equal to zero. However, each of these orders may be regarded as equally standard if a factor $(N_k + 1)^{-1}$ is inserted. Therefore

$$\Delta E' = \sum_{n=1}^{\infty} \sum_{k_1 + \cdots + k_{n-1} = n-1}^{k_i \geq 0} (N_k + 1)^{-1} \left\langle J_o' \middle| H_1 \mathcal{G}_{k_1}^{(')} H_1 \cdots \mathcal{G}_{k_{n-1}}^{(')} H_1 \middle| J_o' \right\rangle . \tag{9.34}$$

Here the factor d'^{-1} and the trace symbol have been eliminated through use of the fact, implied by the non-removability of the degeneracy, that H_1 is diagonal within each subspace $P_0^{(\prime)}$.

Eq. (9.34) is known as the Rayleigh-Schrödinger perturbation formula. Its consistency with expansions (9.13, 14) may be checked directly by substituting it, together with the diagonal elements of these expansions, into the equation $\left\langle J_o' \middle| \Delta^{(\prime)} \middle| J_o' \right\rangle = \Delta E' \left\langle J_o' \middle| \mathfrak{P}^{(\prime)} \middle| J_o' \right\rangle$ and making a term by term comparison on either side.

<u>Connection with the adiabatic switching formalism.</u>

The formulae obtained thus far have been based on a technique of contour integration which has little apparent connection with the theoretical treatment of the perturbation problem given in section 6, based on the adiabatic switching method. That the connection is closer than first appears, however, may be shown by constructing the operators $\mathfrak{P}^{(\prime)}$ and $\Delta^{(\prime)}$ in the adiabatic formalism and then applying expansion (5.5).

The operator $\mathfrak{P}^{(\prime)}$ is given simply by

$$\mathfrak{P}^{(\prime)} = \bar{U}^{ad}(0, \mp\infty)\, P_0^{(\prime)}\, \bar{U}^{ad}(\mp\infty, 0) \quad . \tag{9.35}$$

The operator $\bar{U}^{ad}(0, \mp\infty)$ and its inverse are both present in this expression, so the oscillating phase factors cancel. The form of the operator $\Delta^{(\prime)}$ follows from Eqs. (6.28), (9.12) and (9.35):

$$\begin{aligned} \Delta^{(\prime)} &= \bar{U}^{ad}(0, \mp\infty)\, \Delta H_o\, P_0^{(\prime)}\, \bar{U}^{ad}(\mp\infty, 0) \\ &= \pm i\epsilon g \left[\partial \bar{U}^{ad}(0, \mp\infty)/\partial g\right] P_0^{(\prime)}\, \bar{U}^{ad}(\mp\infty, 0) \quad . \end{aligned} \tag{9.36}$$

Insertion of expansion (5.5) into Eqs. (9.35, 36) leads to power series expansions of $\mathfrak{P}^{(\prime)}$ and $\Delta^{(\prime)}$, of which the <u>n</u>th order terms are given

respectively by*

$$P_n^{(\prime)} = \sum_{m=0}^{n} \frac{1}{H_o' - H_o \pm im\epsilon} H_1 \cdots \frac{1}{H_o' - H_o \pm i\epsilon} H_1 P_0^{(\prime)} H_1 \frac{1}{H_o' - H_o \mp i\epsilon} \cdots H_1 \frac{1}{H_o' - H_o \mp i(n-m)\epsilon} , \tag{9.37}$$

$$\Delta_n^{(\prime)} = \sum_{m=1}^{n} \pm i\, m\epsilon \frac{1}{H_o' - H_o \pm im\epsilon} H_1 \cdots \frac{1}{H_o' - H_o \pm i\epsilon} H_1 P_0^{(\prime)} H_1 \frac{1}{H_o' - H_o \mp i\epsilon} \cdots H_1 \frac{1}{H_o' - H_o \mp i(n-m)\epsilon} . \tag{9.38}$$

Expressions (9.37, 38) can be replaced by contour integrals:

$$P_n^{(\prime)} = (2\pi i)^{-1} \oint_{C'} \frac{1}{E - H_o \pm i\, n\epsilon} H_1 \cdots \frac{1}{E - H_o \pm i\epsilon} H_1 \frac{1}{E - H_o} dE , \tag{9.39}$$

$$\Delta_n^{(\prime)} = (2\pi i)^{-1} \oint_{C'} (E - H_o' \pm i\, n\epsilon) \frac{1}{E - H_o \pm in\epsilon} H_1 \cdots \frac{1}{E - H_o \pm i\epsilon} H_1 \frac{1}{E - H_o} dE . \tag{9.40}$$

Here each contour C' consists of a pair of lines paralleling the imaginary axis and straddling the sequence of poles at H_o', $H_o' \pm i\epsilon$, $H_o' \pm 2i\epsilon$, ...**

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* It is to be noted that the E' in Eq. (5.5) are the levels of the reference system H_o and should be replaced by H_o' here.

** The occurrence of such infinite sequences of poles along the lines $\mathrm{Re}\, E = H_o'$ is characteristic of adiabatic switching. The even spacing of the poles, however, is not a general feature, being merely a peculiarity of the exponential damping factor $e^{-\epsilon|t|}$.

In the limit $\epsilon \to 0$ Eqs. (9.39, 40) reduce to (9.13b, 14b), q.e.d. The identity of $|\alpha_+'\rangle$ and $|\alpha_-'\rangle$ in the bound state case becomes thereby incidentally evident.

A direct expansion of the level shifts themselves may be obtained from Eq. (6.28). It is easy to show that [41]

$$\left\langle J_o'' \middle| \Delta H_o \middle| J_o' \right\rangle = \sum_{n=1}^{\infty} \frac{\pm i\epsilon}{H_o' - H_o'' \pm in\epsilon} \left\langle J_o'' \middle| \left[\bar{U}^{ad}(\mp\infty, 0) H_1 \bar{U}^{ad}(0, \mp\infty) \right]_n \middle| J_o' \right\rangle \tag{9.41}$$

where the notation $[\quad]_n$ picks out the nth order term of a given quantity, and hence that

$$\Delta E_n' = n^{-1} \left\langle J_o' \middle| \left[\bar{U}^{ad}(\mp\infty, 0) H_1 \bar{U}^{ad}(0, \mp\infty) \right]_n \middle| J_o' \right\rangle . \tag{9.42}$$

This equation implies

$$g\, \partial \Delta E'/\partial g = \left\langle J' \middle| H_1 \middle| J' \right\rangle . \tag{9.43}$$

One may verify by direct computation that the Rayleigh-Schrödinger formula is obtainable, when no degeneracy is removed, by writing

$$\frac{1}{H_o' - H_o \pm im\epsilon} = \frac{P_o^{(')}}{\pm im\epsilon} \quad \frac{1 - P_o^{(')}}{H_o' - H_o} \left(1 + \frac{\pm im}{H_o' - H_o} \right)^{-1} , \tag{9.44}$$

expanding and inserting this into (9.42), and discarding terms of orders ϵ , ϵ^2, ... etc.

Convergence of the series expansions.

If, for a given unperturbed level H_0', the expansions (9.13), (9.14) and (9.34) converge at all, they define functions of g which are not only continuous along the real axis but also analytic in the complex plane in the neighborhood of $g = 0$. Thus far we have tacitly assumed that these expansions converge for real values of g small enough so that no perturbed levels cross over a suitable contour C' surrounding H_0'. It is easy to see that this condition, when generalized to include complex values of g, does, in fact, determine a lower bound to the radius of convergence of the expansions, and that the possibility of a convergence failure occurs simultaneously with a failure of the binomial expansion of (9.2) to converge everywhere on the contour in question.

For $g = 0$ the energy levels lie on the real axis in the complex E-plane. For finite $|g|$ the positions of the levels will describe closed curves intersecting the real axis as the phase of g changes from 0 to 2π. A plot of the level structure in $(E, |g|)$-space therefore consists of cones having their vertices in the plane $|g| = 0$ at the eigenvalues of H_0. Consider the cone emmanating from the point $(H_0', 0)$, together with its adjacent neighbors. Intersect these cones by a plane $|g| = r > 0$ and project the portions of the cones lying below this plane onto the plane $|g| = 0$. A lower bound to the radius of convergence of the expansions corresponding to the level H_0' is then given by the largest value of r for which these projections do not overlap one another. This may be seen by choosing the contour C' so as to surround the maximum projection containing H_0' without intersecting the adjacent maximum projections more than tangentially. (C' may, if desired, be left open in the imaginary direction so as to accommodate the situation arising in Eqs. (9.39, 40).)

If now $|g|$ is increased beyond the value r_{max} at which overlap occurs, the integrals (9.9, 10) will, for some complex phase of g, suffer abrupt changes of value arising from the fact that one of the levels has crossed over C'. At the value of g for which the crossover occurs the operator function G(E) has a singularity on C'. This singularity must reflect itself in a convergence failure of the binomial expansion of (9.2).

For $|g| < r_{max}$, the functions $\mathfrak{P}^{(')}$, $\Delta^{(')}$, $\Delta E'$ have no singularities or other peculiarities. Therefore if their expansions converge at all they must converge in this region. The actual radius of convergence is frequently r_{max} itself, although this is not necessarily so, since r_{max} is only a lower bound for it. A trivial example for which r_{max} is <u>not</u> the convergence radius is afforded by the case in which H_1 commutes with H_0. The level shifts in this case depend linearly on g and the radius of convergence is infinite regardless of how much the perturbed levels cross one another. Thus although the binomial expansion of (9.2), and hence the method of deriving the expansion formulae (9.13, 14) etc., breaks down at $|g| = r_{max}$, the formulae themselves may occasionally have a wider range of validity.

Kato [56] has derived a simple theorem which provides a lower bound to r_{max} when none of the properties of the perturbation H_1 are known except its <u>norm</u>. The norm $|F|$ of an operator F is defined by

$$|F| \equiv \max \langle \psi | F^* F | \psi \rangle^{\frac{1}{2}} \quad \text{for all normalized vectors } |\psi\rangle . \tag{9.45}$$

If F is Hermitian its norm is the magnitude of its largest eigenvalue. Norms satisfy the inequalities

$$|F + G| \leq |F| + |G| , \qquad |F\,G| \leq |F|\,|G| . \tag{9.46}$$

Now let the contour C' consist of two lines parallel to the imaginary axis, straddling the point H_0' at a distance $\frac{1}{2}\omega'$, where ω' is the distance of H_0' from the nearest adjacent level. Then

$$\left|G_0(E)\right| \leqslant 2/\omega' \qquad \text{for } E \text{ on } C' , \tag{9.47}$$

and convergence of the binomial expansion of (9.2) is assured if

$$g < \tfrac{1}{2}\,\omega'/|V| \quad , \tag{9.48}$$

where $H_1 = gV$, so that

$$\left|H_1\, G_0(E)\right| \leqslant g\,|V|\,\left|G_0(E)\right| < 1 \quad . \tag{9.49}$$

The quantity $\frac{1}{2}\omega'/|V|$ is the lower bound to r_{max}, and condition (9.48) quarantees the convergence of the Rayleigh-Schrödinger perturbation formula.

Alternative formulations

Because the Rayleigh-Schrödinger formula is a direct and unsophisticated expansion in powers of g it has the poorest rate of convergence possible. It is therefore desirable to seek other computational techniques. Eq. (6.8) provides as good a starting point as any. We first note that this equation can be written in the form

$$Z'^{\frac{1}{2}}\left|J'\right\rangle = \left|J_0'\right\rangle + Z'^{\frac{1}{2}}\,\frac{1}{E' - \mathcal{H}_0 \pm i\epsilon}\,\mathcal{H}_1\left|J'\right\rangle \tag{9.50}$$

which is the generalization of Eq. (7.7). Multiplying (9.50) on the left by $\left\langle J_0'\right|$, and taking note of the limit $\epsilon \to 0$, one infers

$$\left\langle J_0'\right|\mathcal{H}_1\left|J'\right\rangle = \pm i\epsilon\, Z'^{-\frac{1}{2}}(Z'-1) \longrightarrow 0 \tag{9.51}$$

which implies

$$\Delta E' = Z'^{-\frac{1}{2}} \left\langle J_o' \middle| H_1 \middle| J' \right\rangle . \tag{9.52}$$

We now assume that removable degeneracy is absent. The operators $P_0^{(')} \mathfrak{B}^{(')} P_0^{(')}$ are then diagonal in the $\left| J_o' \right\rangle$, and Eq. (9.51) may be generalized to

$$P_0^{(')} \mathcal{H}_1 \left| J' \right\rangle = \pm i \epsilon Z'^{-\frac{1}{2}} (Z' - 1) \left| J_o' \right\rangle \tag{9.53}$$

so that Eq. (9.50) may be rewritten in the form

$$Z'^{-\frac{1}{2}} \left| J' \right\rangle = \left| J_o' \right\rangle + Z'^{-\frac{1}{2}} \frac{1 - P_0^{(')}}{E' - \mathcal{H}_o} \mathcal{H}_1 \left| J' \right\rangle . \tag{9.54}$$

The factor $1 - P_0^{(')}$ in the second term on the right allows the limit $\epsilon \rightarrow 0$ to be taken at once, the superfluousness of the $\pm$ signs becoming again evident. A more useful form of Eq. (9.54) may be obtained by observing that

$$\frac{1 - P_0^{(')}}{E' - \mathcal{H}_o} = \frac{1 - P_0^{(')}}{E' - H_o} \left(1 + \frac{\Delta H_o}{E' - \mathcal{H}_o} \right) , \tag{9.55}$$

which yields

$$\begin{aligned} Z'^{-\frac{1}{2}} \left| J' \right\rangle &= \left| J_o' \right\rangle + Z'^{-\frac{1}{2}} \frac{1 - P_0^{(')}}{E' - H_o} \mathcal{H}_1 \left| J' \right\rangle \\ &\quad + \frac{1 - P_0^{(')}}{E' - H_o} \Delta H_o \; Z'^{-\frac{1}{2}} \left(\left| J' \right\rangle - \left| J_o' \right\rangle \right) \\ &= (1 - g\, M^{(')})^{-1} \left| J_o' \right\rangle \end{aligned} \tag{9.56}$$

where

$$M^{(\prime)} = \frac{1 - P_0^{(\prime)}}{E' - H_o} V \tag{9.57}$$

Substitution of (9.56) into (9.52) then gives an equation for the shifted levels:

$$E' = H_o' + \left\langle J_o' \middle| H_1 \left(1 - \frac{1 - P_0^{(\prime)}}{E' - H_o} H_1 \right)^{-1} \middle| J_o' \right\rangle . \tag{9.58}$$

Still another formulation can be obtained through use of the relation

$$\frac{1 - P_0^{(\prime)}}{E' - H_o} = \frac{1 - P_0^{(\prime)}}{H_o' - H_o} \left(1 - \frac{\Delta E'}{E' - H_o} \right) \tag{9.59}$$

in Eq. (9.56). This yields

$$Z'^{-\frac{1}{2}} \left| J' \right\rangle = \left| J_o' \right\rangle + Z'^{-\frac{1}{2}} \frac{1 - P_0^{(\prime)}}{H_o' - H_o} H_1 \left| J' \right\rangle$$

$$- \frac{1 - P_0^{(\prime)}}{H_o' - H_o} \Delta E' \left(Z'^{-\frac{1}{2}} \left| J' \right\rangle - \left| J_o' \right\rangle \right)$$

$$= \left(1 - g\, N^{(\prime)} \right)^{-1} \left| J_o' \right\rangle \tag{9.60}$$

where

$$N^{(\prime)} = \frac{1 - P_0^{(\prime)}}{H_o' - H_o} \left(H_1 - \Delta E' \right) . \tag{9.61}$$

The level shift equation is

$$\left\langle J_o' \middle| (H_1 - \Delta E') \left[1 - \frac{1 - P_0^{(\prime)}}{H_o' - H_o} (H_1 - \Delta E') \right]^{-1} \middle| J_o' \right\rangle = 0 . \tag{9.62}$$

Any attempt to solve Eqs. (9.58) or (9.62) for the level shifts in powers of g will lead to the Rayleigh-Schrödinger formula. However, there is no need to solve them in this way, for the possibility is now open of obtaining <u>iterative</u> solutions which have a better rate of convergence. For example, Eq. (9.58) is comprehended in the iterative scheme

$$E' = \lim_{n\to\infty} E_n' \quad , \qquad E_o' = H_o' \quad ,$$
$$E_n' = H_o' + \sum_{m=0}^{n-1} \left\langle J_o' \right| H_1 \left(\frac{1 - P_0^{(')}}{E_{n-1}' - H_o} H_1 \right)^m \left| J_o' \right\rangle \quad . \tag{9.63}$$

An improved version of this scheme, which consists of a regrouping of terms in such a manner that a given matrix element of H_1 appears only once in a given term of the sum in (9.63), has been given by Feenberg[53 to 55].

Although these iterative schemes generally provide a more rapid <u>rate</u> of convergence than the Rayleigh-Schrödinger formula, the actual convergence is still limited. However, the limiting factor is now the radius of convergence of the binomial expansion of (9.58) and (9.62), and, as will presently become apparent, this can often be larger than r_{max}. We shall restrict the discussion to Eq. (9.58) and the operator $M^{(')}$, as identical remarks may be applied to Eq. (9.62) and the operator $N^{(')}$.

The radius of convergence of the binomial expansion of (9.58) is the absolute value of the smallest g for which the operator $gM^{(')}$ has unity as one of its eigenvalues. Or, said in another way, it is the reciprocal of the magnitude of the largest eigenvalue of $M^{(')}$. Denote this largest eigenvalue by g'^{-1} and the corresponding eigenvector by $|\psi'\rangle$. Then

$$g' M^{(')} |\psi'\rangle = |\psi'\rangle \tag{9.64}$$

or

$$(E' - H_0)\,|\psi'\rangle = (1 - P_0^{(')})\,H_1\,|\psi'\rangle \tag{9.65}$$

where $H_1 = g'V$. It is evident that $|\psi'\rangle$ is orthogonal to the subspace $P_0^{(')}$. Such a vector arises naturally when g takes on a value for which an accidental degeneracy occurs due to a crossover of the level E' with another level which came originally (at $g = 0$) from a different position H_0'', $H_0'' \neq H_0'$. Denote by $|J''\rangle$ the vector from the subspace $\mathfrak{B}^{('')}$ which corresponds to $|J'\rangle$ in $\mathfrak{B}^{(')}$. Both $|J''\rangle$ and $|J'\rangle$ will generally contain the vector $|J_0'\rangle$ as a component. However, a suitable linear combination of $|J''\rangle$ and $|J'\rangle$ can be found which has no components from $P_0^{(')}$ and which is an eigenvector of H when the crossover in question occurs. This is the vector $|\psi'\rangle$.

The reciprocal eigenvalue g' is therefore generally the smallest value of g for which a crossover takes place between E' and another, originally distinct, level. It is clear that such an actual coalescing of levels may possibly not occur until a much larger value of $|g|$ is reached than that for which a mere overlap of the cone projections previously considered occurs. Thus $|g'|$ will frequently be larger than r_{max}, but never smaller. It is to be noted that g' may be complex since the operator $M^{(')}$ is not generally Hermitian.

<u>The Fredholm method.</u>

The expression $(1 - g\,M^{(')})^{-1}$ has singularities at all the reciprocal eigenvalues of $M^{(')}$. An analytic continuation which bypasses these singularities and therefore eliminates all restrictions on convergence is provided by the Fredholm method. We shall content ourselves here with

a mere statement of the Fredholm formula and refer the reader to standard works for details (e.g. reference [10], p. 1018 ff.).

One rewrites Eq. (9.58) in the form

$$E' = H_o' + \left\langle J_o' \middle| H_1 \, Q^{(')}/D^{(')} \middle| J_o' \right\rangle \tag{9.66}$$

where

$$D^{(')} = \exp\left[- \int_0^g \mathrm{Tr}\, g^{n-1} M^{(')n} (1 - g\, M^{(')})^{-1} \, dg \right] \tag{9.67a}$$

$$= \exp \int_0^g \sum_i (g/g_i)^{n-1} (g - g_i)^{-1} \, dg \tag{9.67b}$$

and

$$Q^{(')} = D^{(')} (1 - g\, M^{(')})^{-1} \quad . \tag{9.68}$$

Here the g_i are the reciprocal eigenvalues of $M^{(')}$ and n is the smallest exponent for which $\mathrm{Tr}\, M^{(')n}$ is finite.

$D^{(')}$ is an entire function of g having zeros at the poles of $(1 - g\, M^{(')})^{-1}$. The operator $Q^{(')}$ is therefore also an entire function of g, and one may carry out an expansion of (9.67a) in powers of g, insert this into (9.68), and carry out the expansion of $Q^{(')}$, knowing that both expansions will converge no matter how large g is.* The ratio of the two expansions is then used directly in (9.66).

Eq. (9.66) has still to be solved for the shifted energy level E'. For this purpose iterative techniques may be used as before. If other methods (graphical ones, for example) are used then care must be taken, since (9.66) may have many different solutions. It is necessary to choose that solution which passes continuously to the value H_o' as g goes to zero.

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* Closed expressions for the coefficients involved are given in reference [10].

The adiabatic theorem.

The adiabatic theorem may be regarded as having been in a sense proved by the demonstration in the present section of the equivalence of the adiabatic constructions of section 6 to other more straightforward perturbation techniques. It is useful, however, to have a proof of this theorem in its most general form, as stated in section 6, in which the adiabatic switching is not restricted to the very special type expressed by Eq. (5.1).

The pattern of proof is classic.[63] One introduces a time dependent Hamiltonian operator $H(t)$ and a set of corresponding eigenvectors $\left| J'(t) \right\rangle$:

$$H(t) \left| J'(t) \right\rangle = E'(t) \left| J'(t) \right\rangle , \tag{9.69}$$

$$\left\langle J''(t) \middle| J'(t) \right\rangle = \delta_{J''J'} . \tag{9.70}$$

Setting $J'' = J'$ in (9.70) and differentiating with respect to the time one sees that $\left\langle J'(t) \middle| (d \left| J'(t) \right\rangle /dt) \right.$ is pure imaginary. Evidently the phases of the eigenvectors can be adjusted so that

$$\left\langle J'(t) \middle| (d \left| J'(t) \right\rangle /dt) \right. = 0 , \tag{9.71}$$

and we shall assume this has been done.

Consider now a Schrödinger state vector of the form

$$\left| \psi(t) \right\rangle = \sum{}' e^{-i \int_0^t E'(t')dt'} A'(t) \left| J'(t) \right\rangle . \tag{9.72}$$

Substitution of this into the Schrödinger equation (1.18) and multiplication of the result by $\left\langle J''(t) \right|$ gives the following differential equation for the amplitudes $A'(t)$:

$$\mathring{A}''(t) = -\sum{}' e^{i\int_0^t \left[E''(t') - E'(t')\right] dt'} A'(t) \left\langle J''(t) \middle| (d \middle| J'(t)\rangle /dt) \right. . \tag{9.73}$$

On the other hand, multiplication of the time derivative of Eq. (9.69) by $\left\langle J''(t)\right|$ gives*

$$\left\langle J''(t) \middle| \mathring{H}(t) \middle| J'(t)\right\rangle + \left[E''(t) - E'(t)\right] \left\langle J''(t) \middle| (d \middle| J'(t)\rangle /dt) \right. = \delta_{J''J'} \dot{E}'(t), \tag{9.74}$$

and hence, in virtue of (9.71),

$$\mathring{A}''(t) = \sum_{J' \neq J''}{}' e^{i\int_0^t \left[E''(t') - E'(t')\right] dt'} A'(t) \frac{\left\langle J''(t) \middle| \mathring{H}(t) \middle| J'(t)\right\rangle}{E''(t) - E'(t)} . \tag{9.75}$$

If $H(t)$ varies slowly with time then its eigenvalues $E'(t)$ vary slowly, and an integral of the form

$$\int_0^t f(t)\, e^{i\int_0^t \left[E''(t') - E'(t')\right] dt'} dt ,$$

where $f(t)$ is also slowly varying, is of order $\bar{f}/\bar{\omega}$ in magnitude, $\bar{\omega}$ being some average value of the level separation $E''(t) - E'(t)$ in the interval 0 to t, and $\bar{f}$ a corresponding average value of $f(t)$. Therefore, if only one of the amplitudes, say $A'(t)$, is excited at $t = 0$, integration of (9.75) for the other amplitudes gives

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* If the time variation of $H(t)$ is regarded as due to a variation in the coupling constant g, Eq. (9.74) reduces, in the case $J'' = J'$, to Eq. (9.43).

$$A''(t) = O(\epsilon \langle H \rangle / \bar{\omega}^2) \quad , \qquad J'' \neq J' \quad , \tag{9.76}$$

where ϵ is the reciprocal of a length of time over which $H(t)$ undergoes significant changes and $\langle H \rangle$ is a typical off-diagonal matrix element of $H(t)$. The adiabatic limit is expressed by $\epsilon \to 0$.

Eq. (9.76) contains the statement of the adiabatic theorem. It shows that if there is no initial degeneracy in the system, so that all the level separations occurring in the sum (9.75) are finite, none of the other amplitudes gets excited in the adiabatic limit, and the vector $|\psi(t)\rangle$ remains a pure eigenvector of $H(t)$.* On the other hand, if initial degeneracy is present, so that $\bar{\omega} \to 0$, then the amplitudes can become all mixed up, unless the degeneracy remains unremoved, in which case the operator $H(t)$ never has nonvanishing off-diagonal elements connecting states of equal energy and the adiabatic theorem will hold in spite of the degeneracy. Even if the degeneracy is removed by the perturbation, however, the amplitudes can still be prevented from becoming mixed up if the vectors $|J'(t)\rangle$ are chosen in such a way that $d|J'(t)\rangle/dt$ remains of order ϵ as $t \to 0$; for the integral of Eq. (9.73) then becomes of order

$$\epsilon \int_0^t e^{i\int_0^t \xi \epsilon t' \, dt'} dt = O(\epsilon/\xi)^{\frac{1}{2}} \to 0$$

for $J'' \neq J'$, the level separation $E''(t) - E'(t)$ being expressible for $t \lesssim 1/\epsilon$ simply as $\xi \epsilon t$ where ξ is some finite constant. This requirement, when applied to the adiabatic construction (6.12), determines the appropriate choice for the vectors $|\alpha_0'\rangle$ and can evidently be satisfied if the eigenvectors $|\alpha_\pm'\rangle$ are analytic functions of the coupling constant g in the neighborhood of $g = 0$.

* To be completely rigorous one should also show that, for reasonable operators $H(t)$, the sum (9.75) converges for any set of amplitudes satisfying $\sum' |A'(t)|^2 = 1$. (See reference [63].)

The adiabatic construction of eigenvectors can also be carried past any point at which an accidental degeneracy occurs, provided again that the $|J'(t)\rangle$ can be chosen in such a way that $d|J'(t)\rangle/dt$ remains of order ϵ right through the time of degeneracy. This condition evidently imposes certain restrictions on the temporal behavior of the operator $H(t)$, but these are of the mildest sort and may usually be ignored.*

The fact that any stage in the switching process the vector $|\psi(t)\rangle$ is an eigenvector of the total Hamiltonian operator for that stage is consistent with Eq. (5.5) which shows that if t and ϵ are allowed to tend respectively to $\mp\infty$ and 0 in such a way that $\epsilon|t|$ remains equal to $-\ln x$, $0 < x < 1$, the result of applying $e^{-iH_0t}\,\bar{U}^{ad}(t,\mp\infty)$ to $|\alpha_0'\rangle$ is to obtain an eigenvector of the operator $H_0 + xH_1$.

<u>The creation of bound states from free states.</u>

An interesting supplement to the adiabatic switching procedure is suggested by the situation occurring in systems which possess both bound and free states, and typically by the situation depicted in Fig. 7, in

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* The type of behavior which is <u>not</u> allowed is illustrated by the simple example

$$H(t) = \begin{cases} \begin{pmatrix} 1 & \epsilon(t-t_0) \\ \epsilon(t-t_0) & 1 \end{pmatrix}, & t < t_0, \\ \begin{pmatrix} 1+\epsilon(t-t_0) & 0 \\ 0 & 1-\epsilon(t-t_0) \end{pmatrix}, & t > t_0. \end{cases}$$

Here although $H(t)$ is a continuous slowly varying function of t, its eigenvectors change abruptly at the time of degeneracy $t = t_0$.

which system H has bound states which have no counterparts in H_0. Although it has been previously remarked that perturbation theory cannot be applied directly to the construction of the eigenvectors for the "extra" states, and that independent and generally more difficult means of construction must be found, one nevertheless suspects that these states ought to be obtainable by some sort of adiabatic process of "peeling them off the bottom of the deck" of higher lying continuum states. It is actually possible to test this conjecture in a simple case.

Before becoming specific let us first consider some of the general features which we should expect to characterize the results of such a procedure. Let the zero point of energy be taken at the bottom of the continuous part of the spectrum. The lowest lying continuum state of the system H_0 will generally be nondegenerate (ignoring nonclassical degrees of freedom), and we shall denote it by $|0\rangle$. If H_0 is a function only of the absolute value of a momentum $\underset{\sim}{p}$, this state will correspond to $\underset{\sim}{p} = 0$.

$$H_0(0) = 0 \quad . \tag{9.77}$$

In case the lower bound of the continuum is itself not included in the spectrum it is necessary to regard $|0\rangle$ as a superposition of states from an infinitesimally thin shell of levels at the bottom, but this does not alter the following discussion.

We wish to consider the effect of applying the operator $\bar{U}^{ad}(0, \mp\infty)$ to $|0\rangle$. If our conjecture is correct then we should obtain a result of the form

$$\bar{U}^{ad}(0, \mp\infty)\,|0\rangle = |0\rangle + \sum{}' A_{\pm}{}' \,|j'\rangle \tag{9.78}$$

where the $|J'\rangle$ are the "extra" bound states. The question arises as to the form and magnitude of the amplitudes $A_\pm'$.

If the perturbation H_1 is a position dependent potential $V(\underset{\sim}{r})$, then the coordinate representation of a given $|J'\rangle$ must, in the region outside the range of the potential, have the form

$$\langle \underset{\sim}{r} | J' \rangle \sim (d^N \underset{\sim}{r})^{\frac{1}{2}} C'^{\frac{1}{2}} e^{-\mu' r} \tag{9.79}$$

where C' is a normalizing constant and

$$H_0(i\mu') = E' < 0 \; ; \tag{9.80}$$

E' being the energy of the state $|J'\rangle$. In this state the coordinate of the system (particle) is more or less certain to be found within a distance of order $\mu'^{-1} + d$ from the origin, where d is the range of the potential (which is assumed to be centered on the origin). On the other hand, in the unperturbed state $|0\rangle$ the coordinate has an equal chance of being anywhere in the fundamental box of side L. The chance of catching the system in the bound state $|J'\rangle$ by switching on the perturbation is therefore of the order of $(\mu'^{-1} + d)^N L^{-N}$, and the amplitude $A_\pm'$ is expected to be proportional to $(\mu'^{-1} + d)^{N/2} L^{-N/2}$. Since a level shift of amount E' is also involved $A_\pm'$ should have as an additional factor a rapidly oscillating phase. Summing up, we expect

$$A_\pm' = f_\pm'(\epsilon)(\mu'^{-1} + d)^{N/2} L^{-N/2} \exp\left[(\pm i\epsilon)^{-1} \int_0^g E'(g)\, g^{-1}\, dg\right] , \tag{9.81}$$

where the $f_\pm'(\epsilon)$ are weight factors which depend on the detailed structure of the system and which may also be expected to depend on the rapidity ϵ with which the perturbation is switched on, though in a much

less singular fashion than the oscillating phase.

Eq. (9.81) will now be verified for the case of the one-dimensional delta-function potential considered at the end of the previous section. Here there is only one bound state, and $d = 0$, $\mu' = g$, $E' = -\frac{1}{2} g^2$. Hence we expect

$$A_{\pm}' = f_{\pm}(\epsilon)\,(gL)^{-\frac{1}{2}}\, e^{\pm\frac{1}{4} i g^2/\epsilon} \tag{9.82}$$

Using Eqs. (5.5), (8.102) and (8.103), we first get

$$\left\langle \underset{\sim}{p}' \middle| \bar{U}^{ad}(0, \mp\infty) \middle| 0 \right\rangle = \delta_{\underset{\sim}{p}'0} + \frac{2g}{L} \sum_{n=0}^{\infty} \frac{1}{p'^2 \mp i\, 2(n+1)\epsilon} \frac{1}{\sqrt{n!}} \left(\frac{\pm i g^2}{2\epsilon}\right)^{\frac{n}{2}}$$

$$= \delta_{\underset{\sim}{p}'0} + \frac{2g}{L} \sum_{m=0}^{\infty} \left\{ \frac{1}{p'^2 \mp i\, 2(2m+1)\epsilon} \frac{1}{\sqrt{(2m)!}} \left(\frac{\pm i g^2}{2\epsilon}\right)^{m} \right.$$

$$\left. + \frac{1}{p'^2 \mp i\, 2(2m+2)\epsilon} \frac{1}{\sqrt{(2m+1)!}} \left(\frac{\pm i g^2}{2\epsilon}\right)^{m+\frac{1}{2}} \right\} . \tag{9.83}$$

For very small ϵ the terms of the above series which give the most important contributions are those for which m is of order $\frac{1}{4} g^2/\epsilon$. Hence the Stirling approximation for the factorial may be used

$$x! \sim \sqrt{2\pi}\; x^{x+\frac{1}{2}}\; e^{-x} , \tag{9.84}$$

giving

$$\sqrt{(2m)!} \sim (2\pi)^{-\frac{1}{4}} 2^{m+\frac{1}{4}} m^{-\frac{1}{4}} m! \rightarrow \pi^{-\frac{1}{4}} 2^{m} m! (\tfrac{1}{4} g^2/\epsilon)^{-\frac{1}{4}} , \tag{9.85}$$

$$\sqrt{(2m+1)!} \sim (2\pi)^{-\frac{1}{4}} 2^{m+\frac{3}{4}} m^{\frac{1}{4}} m! \rightarrow \pi^{-\frac{1}{4}} 2^{m} \tfrac{1}{2} m! (\tfrac{1}{4} g^2/\epsilon)^{\frac{1}{4}} . \tag{9.86}$$

In the final forms of Eqs. (9.85, 86) the extra factor $m^{\pm\frac{1}{4}}$ has been replaced by its "peak value" $(\frac{1}{4} g^2/\epsilon)^{\pm\frac{1}{4}}$, in recognition of the fact that the fractional width of the group of significant terms of the series (9.83) becomes smaller and smaller as ϵ tends to zero. Therefore, for very small ϵ

$$\left\langle \underset{\sim}{p'} \middle| \bar{U}^{ad}(0, \mp\infty) \middle| 0 \right\rangle = \delta_{\underset{\sim}{p'}0} + f_{\pm}(\epsilon) \frac{2g}{L} \sum_{m=0}^{\infty} \frac{1}{p'^2 \mp i\, 4m\epsilon} \frac{1}{m!} \left(\frac{\pm i\, g^2}{4\epsilon} \right)^m , \tag{9.87}$$

where

$$f_{\pm}(\epsilon) = (1 + e^{\pm i\pi/4}) (\tfrac{1}{4} \pi g^2/\epsilon)^{\frac{1}{4}} . \tag{9.88}$$

If it were not for the presence of the factor $(p'^2 \mp i\, 4\, m\epsilon)^{-1}$, (9.87) would be the series for $\exp(\pm \frac{1}{4} i\, g^2/\epsilon)$. However, this exponential can be maintained as a factor if we expand $(p'^2 \mp i\, 4\, m)^{-1}$ in powers of p'^{-2} and make use of the asymptotic relation

$$(-g^2/p'^2)^s e^{\pm\frac{1}{4} i\, g^2/\epsilon} \sim (\pm i\, 4\epsilon/p'^2)^s (-\epsilon\, \partial/\partial\epsilon)^s e^{\pm\frac{1}{4} i\, g^2/\epsilon}$$

$$= \sum_{m=0}^{\infty} \left(\frac{\pm i\, 4\, m\epsilon}{p'^2} \right)^s \frac{1}{m!} \left(\frac{\pm i\, g^2}{4\epsilon} \right)^m . \tag{9.89}$$

When m is near its "peak value" the expansion of $(p'^2 \mp i\, 4\, m\epsilon)^{-1}$ converges

in the same region as expansion (8.104), namely for $p' > g$, and may be analytically continued to smaller values of p'. Hence we write

$$\sum_{m=0}^{\infty} \frac{1}{p'^2 \mp i\, 4m\epsilon} \frac{1}{m!} \left(\frac{\pm i\, g^2}{4\epsilon}\right)^m = \sum_{m=0}^{\infty} \sum_{s=0}^{\infty} \frac{1}{p'^2} \left(\frac{\pm i\, 4m\epsilon}{p'^2}\right)^s \frac{1}{m!} \left(\frac{\pm i g^2}{4\epsilon}\right)^m$$

$$\sim \sum_{s=0}^{\infty} p'^{-2} (-g^2/p'^2)^s\, e^{\pm \frac{1}{4} i\, g^2/\epsilon} = (g^2 + p'^2)^{-1}\, e^{\pm \frac{1}{4} i\, g^2/\epsilon} , \tag{9.90}$$

which, in virtue of (8.100), leads to (9.82) with the function $f_{\pm}(\epsilon)$ given by (9.88). In deriving expression (9.90) we have, of course, left many of the important mathematical steps unjustified, such as the reckless use of the asymptotic forms, interchange of orders of summation, etc. The derivation can, however, be made rigorous through the use of proper analytical techniques.

It may perhaps seem surprising that $f_{\pm}(\epsilon)$ turns out to be a singular function of ϵ at the origin. The singularity is, however, a weak one $(\sim \epsilon^{-\frac{1}{4}})$, and, since condition (7.18) must always hold,

$$\lim_{\epsilon \to 0} A_{\pm}' = 0 . \tag{9.91}$$

This means that even though the bound state can be adiabatically created from the continuum it never has more than a transitory existence when constructed in this way. This conclusion should hold generally for all systems.

10. SIMPLE FIELD THEORIES

The nonrelativistic extended source model.

The most striking of the special problems posed by field theories, namely the problem of the renormalization of constants, can be illustrated by relatively simple examples. In this section we shall consider systems having Hamiltonian operators of the general form*

$$H = \int \psi^* M_o \psi \, d^3\underset{\sim}{r} + \tfrac{1}{2} \sum_A \int \left[\pi_A^{\,2} + (\nabla \phi_A)^2 + \mu_o^{\,2} \phi_A^{\,2} \right] d^3\underset{\sim}{r} - E_{vac}$$
$$+ g \sum_{j,A} \int d^3\underset{\sim}{r} \int d^3\underset{\sim}{r} \, \phi_A' \, \rho_j(\underset{\sim}{r}' - \underset{\sim}{r}) \psi^* T_{jA} \psi \, . \tag{10.1}$$

Here we use the abbreviations

$$\psi = \psi(\underset{\sim}{r}) \, , \qquad \phi_A = \phi_A(\underset{\sim}{r}) \, , \qquad \phi_A' = \phi_A(\underset{\sim}{r}') , \qquad \text{etc.} \tag{10.2}$$

The field ψ may have several components ψ_μ, and the notation contained in Eq. (10.1) is then to be understood as involving matrix-vector multiplication. If the basic commutation relations are taken as**

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* This form may be derived from the Lagrangian density

$$\mathcal{L} = i \underset{\sim}{\psi}^* (\dot{\underset{\sim}{\psi}} + i M_o \underset{\sim}{\psi}) - \tfrac{1}{2} \sum_A \left[(\nabla \underset{\sim}{\phi}_A)^2 - \dot{\underset{\sim}{\phi}}_A^{\,2} + \mu_o^{\,2} \underset{\sim}{\phi}_A^{\,2} \right] + L^{-3} E_{vac}$$
$$- g \sum_{j,A} \int \underset{\sim}{\phi}_A' \, \rho_j(\underset{\sim}{r}' - \underset{\sim}{r}) \underset{\sim}{\psi}^* T_{jA} \underset{\sim}{\psi} \, d^3\underset{\sim}{r}' \, ,$$

which yields the equations of motion in the Heisenberg representation:

$$\dot{\underset{\sim}{\psi}} + i \left\{ M_o + g \sum_{j,A} \left[\int \underset{\sim}{\phi}_A' \, \rho_j(\underset{\sim}{r}' - \underset{\sim}{r}) d^3\underset{\sim}{r}' \right] T_{jA} \right\} \underset{\sim}{\psi} = 0$$

$$\nabla^2 \underset{\sim}{\phi}_A - \ddot{\underset{\sim}{\phi}}_A - \mu_o^{\,2} \underset{\sim}{\phi}_A = g \sum_j \int \rho_j(\underset{\sim}{r} - \underset{\sim}{r}') \underset{\sim}{\psi}'^* T_{jA} \underset{\sim}{\psi}' \, d^3\underset{\sim}{r}' \, .$$

** The brackets $\{ \; \}$ denote the anticommutator.

$$\left[\phi_A, \pi_B'\right] = i\,\delta_{AB}\,\delta(\underset{\sim}{r} - \underset{\sim}{r}'), \qquad \{\psi_\mu, \psi_\nu'^*\} = \delta_{\mu\nu}\,\delta(\underset{\sim}{r} - \underset{\sim}{r}'),$$

$$\{\psi_\mu, \psi_\nu'\} = \{\psi_\mu^*, \psi_\nu'^*\} = 0, \tag{10.3}$$

with the commutators of all other pairs of field quantities vanishing, then the ψ_μ describe <u>fixed fermion sources</u> of a set of real scalar (or pseudo-scalar) <u>boson</u> fields ϕ_A. Following custom we shall refer to the fermions as <u>nucleons</u> and to the bosons as <u>mesons</u>.

The last term of (10.1) is generally called the "coupling term," g being the coupling constant. The Hamiltonian operator H_0 of the "natural" reference system is obtained by setting $g = 0$, and involves only the quantities M_0 and μ_0, the "bare" nucleon and meson masses respectively. The constant E_{vac} is inserted merely for convenience to cancel the vacuum oscillation energy so that the vacuum state will define the zero point of energy. In relativistic field theories the masses of the <u>real</u> nucleon and meson when $g \neq 0$, call them M and μ, will generally differ from M_0 and μ_0. The adjustable constant E_{vac} must also vary with g in order to keep the <u>real</u> vacuum at zero energy. In the present nonrelativistic example, however, only M will depend on g. A g-dependence for μ_0 and E_{vac} requires the possibility of nucleon pair creation, and this will be prohibited by taking M_0 as a simple positive real constant rather than the more general matrix having both negative and positive eigenvalues. As partial compensation for this restriction the nucleons will be allowed to have a finite extension through the presence of the real functions

$\rho_j(\underset{\sim}{r} - \underset{\sim}{r}')$.* These functions give to the meson nucleon interaction a so-called nonlocal character. The remaining features of the interaction are described by a set of Hermitian matrices, the T_{jA}.

A condensed notation.

For practical calculations it is convenient to pass to the momentum representation. The procedure is familiar.** One makes a Fourier analysis of the meson field variables with respect to an enclosing box of volume L^3

$$\varphi_{A,\underset{\sim}{p}} = L^{-3/2} \int \varphi_A(\underset{\sim}{r})\, e^{-\underset{\sim}{p}\cdot\underset{\sim}{r}}\, d^3\underset{\sim}{r} = \varphi_{A,-\underset{\sim}{p}}^{*} , \tag{10.4}$$

$$\pi_{A,\underset{\sim}{p}} = L^{-3/2} \int \pi_A(\underset{\sim}{r}) e^{-\underset{\sim}{p}\cdot\underset{\sim}{r}}\, d^3\underset{\sim}{r} = \pi_{A,-\underset{\sim}{p}}^{*} , \tag{10.5}$$

and then introduces the operators

$$a_{A,\underset{\sim}{p}} = -i(2\omega)^{-\frac{1}{2}} (\pi_{A,\underset{\sim}{p}} - i\omega\varphi_{A,\underset{\sim}{p}}) , \tag{10.6a}$$

$$a_{A,\underset{\sim}{p}}^{*} = -i(2\omega)^{-\frac{1}{2}} (\pi_{A,-\underset{\sim}{p}} + i\omega\varphi_{A,-\underset{\sim}{p}}) , \tag{10.6b}$$

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* Chew (reference [92]) has considered systems of the extended source type from the point of view of renormalization theory. Specifically he has considered the charge symmetric pseudoscalar theory with

$$\rho_j(\underset{\sim}{r} - \underset{\sim}{r}') = \mu_o^{-1}\, \partial\rho(\underset{\sim}{r} - \underset{\sim}{r}')/\partial x_j , \qquad \underset{\sim}{r} = (x_1, x_2, x_3) ,$$

$$\int \rho(\underset{\sim}{r}) d^3\underset{\sim}{r} = 1 , \qquad T_{jA} = \sigma_j \tau_A ,$$

the σ_j and τ_A being the spin and isotopic spin matrices respectively. Much work has been done in the past on systems of this type from the point of view of strong coupling theory. [6] There, however, the splitting of H into a perturbation H_1 and an unperturbed Hamiltonian H_o is done quite differently, and the phenomena of renormalization are for the most part obscured.

** See, for example, reference [7], chap. II, § 6.

where ω is the energy of a meson of momentum $\underset{\sim}{p}$:

$$\omega = (p^2 + \mu^2)^{\frac{1}{2}} , \qquad p = |\underset{\sim}{p}| . \tag{10.7}$$

In order to concentrate on essential features we shall suppress the indices $A, \underset{\sim}{p}$ by introducing an ∞-dimensional Euclidean vector space. Let the members of a set of orthonormal real basis vectors in this space be denoted by $b_{A,\underset{\sim}{p}}$:

$$b_{A,\underset{\sim}{p}} \cdot b_{A',\underset{\sim}{p}'} = \delta_{AA'} \delta_{\underset{\sim}{p}\underset{\sim}{p}'} , \tag{10.8}$$

the dot indicating the scalar product. Then introduce the vectors

$$a = \sum_{A,\underset{\sim}{p}} a_{A,\underset{\sim}{p}} b_{A,\underset{\sim}{p}} , \qquad a^* = \sum_{A,\underset{\sim}{p}} a_{A,\underset{\sim}{p}}^* b_{A,\underset{\sim}{p}} . \tag{10.9}$$

These vectors satisfy the commutation relations

$$\begin{aligned} [a, a] &= [a^*, a^*] = 0 , \\ [a, a^*] &= \sum_{A,\underset{\sim}{p}} b_{A,\underset{\sim}{p}} b_{A,\underset{\sim}{p}} = \underset{\sim}{1}_b , \end{aligned} \tag{10.10}$$

where $\underset{\sim}{1}_b$ denotes the unit dyadic in the space of the $b_{A,\underset{\sim}{p}}$.

It is also convenient to introduce another vector space for the nucleon field variables, with a corresponding set of basic vectors $f_{\mu,\underset{\sim}{r}}$,

$$f_{\mu,\underset{\sim}{r}} \cdot f_{\nu,\underset{\sim}{r}'} = \delta_{\mu\nu} \delta_{\underset{\sim}{r}\underset{\sim}{r}'} , \tag{10.11}$$

and to define

$$\Psi = \sum_{\mu,\underset{\sim}{r}} (d^3\underset{\sim}{r})^{\frac{1}{2}} \psi_\mu(\underset{\sim}{r}) f_{\mu,\underset{\sim}{r}} , \qquad \Psi^* = \sum_{\mu,\underset{\sim}{r}} (d^3\underset{\sim}{r})^{\frac{1}{2}} \psi_\mu^*(\underset{\sim}{r}) f_{\mu,\underset{\sim}{r}} . \tag{10.12}$$

The Ψ's commute with the a's but, among themselves, satisfy the anti-commutation relations

$$\{\Psi, \Psi\} = \{\Psi^*, \Psi^*\} = 0 \quad ,$$
$$\{\Psi, \Psi^*\} = \sum_{\mu,\underset{\sim}{r}} f_{\mu,\underset{\sim}{r}} f_{\mu,\underset{\sim}{r}} = \underset{\sim}{1}_f \quad , \tag{10.13}$$

where $\underset{\sim}{1}_f$ is the unit dyadic in the space of the $f_{\mu,\underset{\sim}{r}}$.

If now the meson field variables in (10.1) are expanded, via (10.4,5,6), in terms of the $a_{A,\underset{\sim}{p}}$, and if the vector notation here introduced is employed, then the Hamiltonian operator reduces to the sum of the two condensed expressions

$$H_o = M_o \Psi^* \cdot \Psi + a^* \cdot \underset{\sim}{\omega} \cdot a \quad , \tag{10.14a}$$

$$H_1 = g \Psi^* \cdot (V_o \cdot a + a^* \cdot V_o^*) \cdot \Psi \, , \tag{10.14b}$$

where

$$\underset{\sim}{\omega} = \sum_{A,\underset{\sim}{p}} b_{A,\underset{\sim}{p}} \, \omega \, b_{A,\underset{\sim}{p}} \quad , \tag{10.15}$$

$$V_o = \sum_{j,A,\underset{\sim}{p},\mu,\nu,\underset{\sim}{r}} (2\omega L^3)^{-\frac{1}{2}} \upsilon_{j,\underset{\sim}{p}} \, e^{i \underset{\sim}{p} \cdot \underset{\sim}{r}} \, f_{\mu,\underset{\sim}{r}} (T_{jA})_{\mu\nu} \, f_{\nu,\underset{\sim}{r}} \, b_{A,\underset{\sim}{p}} \quad , \tag{10.16}$$

$$\upsilon_{j,\underset{\sim}{p}} = \int \rho_j(\underset{\sim}{r}) \, e^{i \underset{\sim}{p} \cdot \underset{\sim}{r}} \, d^3\underset{\sim}{r} = \upsilon_{j,-\underset{\sim}{p}}^* \quad . \tag{10.17}$$

In the passage from (10.1) to (10.14) the vacuum oscillation energy has been removed by setting

$$E_{vac} = \tfrac{1}{2} \, \mathrm{Tr} \, \underset{\sim}{\omega} \quad . \tag{10.18}$$

The matrix-vector multiplication in expression (10.14b) involves, in an obvious fashion, the direct product of the vector space of the b's with that of the f's. The quantity V_o is a vector in b-space and a dyadic in

f-space, and it is known as the simple vertex operator for reasons which will presently become apparent. Its Hermitian adjoint, which is indicated by the asterisk in (10.14b), is to be understood as involving a transposition in f-space as well as a complex conjugation.

The operators a and a^* respectively annihilate and create a meson, and the operators Ψ and Ψ^* do the same for a nucleon. The vacuum state of the reference system H_o is defined as the no-particle state, i.e. the state from which no particles can be removed by the annihilation operators:

$$a \,|\, vac\rangle = 0 \,, \qquad \Psi \,|\, vac\rangle = 0 \,. \tag{10.19}$$

It is evident from the form of the interaction (10.14b) that $|vac\rangle$ is an eigenvector of the total Hamiltonian operator, having the eigenvalue zero.

$$H \,|\, vac\rangle = 0 \,. \tag{10.20}$$

Thus $|vac\rangle$ not only represents the so-called "bare" vacuum of the system H_o but also the real vacuum of the system H. In theories which allow nucleon pair creation the real vacuum state vector is generally different from the bare vacuum state vector.

The bare one-particle states are obtained by applying the creation operators to the vacuum:

$$|\pi_o\rangle = a^* \,|\, vac\rangle \,, \qquad |N_o\rangle = \Psi^* \,|\, vac\rangle \,. \tag{10.21}$$

The quantities $|\pi_o\rangle$ and $|N_o\rangle$ are vectors not only in state-vector space but also respectively in b- and f-space. The state-vector describing a single bare meson of momentum $\underset{\sim}{p}$ in the state A, with no nucleons present, is obtained by taking the scalar product of $b_{A,\underset{\sim}{p}}$ with $|\pi_o\rangle$. Similarly,

the scalar product of $f_{\mu,\underset{\sim}{r}}$ with $|N_o\rangle$ describes a single bare nucleon at the point $\underset{\sim}{r}$ in the state μ .

Since Ψ commutes with a^* it is evident that $\Psi|\pi_o\rangle = 0$, and hence that $|\pi_o\rangle$ is an eigenvector not only of H_o but also of the total Hamiltonian operator:

$$H_o|\pi_o\rangle = H|\pi_o\rangle = |\pi_o\rangle\cdot\underset{\sim}{\omega} \tag{10.22}$$

Therefore the single real meson state, which may be described by a vector $|\pi\rangle$, is identical with the single bare meson state in the present theory:

$$|\pi\rangle = |\pi_o\rangle \tag{10.23}$$

On the other hand, the single real nucleon state, which will be denoted by the vector $|N\rangle$, is not identical with $|N_o\rangle$.

<u>The particle propagation functions</u>

Of fundamental importance in quantum field theories are the expectation values of the Green's functions $G_{0\pm}(E)$ and $G_{\pm}(E)$ in the bare one-particle states. These are known as the unmodified and modified one-particle propagation functions respectively. In the present example the unmodified and modified meson propagation functions are identical:

$$\langle\pi_o|G_{0\pm}(E)|\pi_o\rangle = \langle\pi_o|G_{\pm}(E)|\pi_o\rangle = \frac{\frac{1}{2}b}{E - \underset{\sim}{\omega} \pm i\epsilon} . \tag{10.24}$$

The two corresponding functions for the nucleon are not identical, however, and a principal task in what follows will be the construction of the modified nucleon propagation function.

Before entering into the details of this task it is well to call attention to the fact that the forms of the mathematical structures which

appear in the development of a given quantum field theory depend very largely on the form of the interaction between the fields. Thus, in the present example, the choice of mathematical structures to be employed will be conditioned by the fact that the interaction (10.14b) is linear in the meson field and bilinear in the nucleon field. Although interactions of this type are currently attracting much greater interest than any other, it is to be remembered that other types can in principle exist, each giving rise to its own special formalism. How far the ideas of renormalization (which we shall discuss presently) can be applied in these other cases is an open question. The only other interaction which has been extensively studied, aside from the trivial one which is linear in each field,* is that which is bilinear in both fields. [110] In this case, although the appropriate formalism has its own peculiarities, the renormalization concepts can still be applied, at least if the interaction is nonlocal. About interactions which are still more complicated, e.g. nonlinear metric interactions in gravitational theory, nothing is known.

In the present example the unmodified nucleon propagation function is given by

$$S_{0\pm}(E) = \left\langle N_0 \middle| G_{0\pm}(E) \middle| N_0 \right\rangle = \frac{\underset{\sim}{1}_f}{E - M_0 \pm i\epsilon} . \tag{10.25}$$

The modified nucleon propagation function, which will be denoted by $S_\pm(E)$, may be expressed in a similar form by making use of the following identity:

---

* Both fields must then have the same statistics, i.e. both fermion or both boson.

$$\underset{\sim}{1}_f = \left\langle N_o \middle| G_\pm(E)(E - H \pm i\epsilon) \middle| N_o \right\rangle$$

$$= \left\langle N_o \middle| G_\pm(E) \middle| N_o \right\rangle \cdot \left\langle N_o \middle| (E - H \pm i\epsilon) \middle| N_o \right\rangle + \left\langle N_o \middle| G_\pm(E) \middle| N_o, \pi_o \right\rangle \cdot \left\langle N_o, \pi_o \middle| (E - H \pm i\epsilon) \middle| N_o \right\rangle$$

$$= S_\pm(E)(E - M_o \pm i\epsilon) - g \left\langle N_o \middle| G_\pm(E) \middle| N_o, \pi_o \right\rangle \cdot V_o^* \quad , \tag{10.26}$$

where $\left| N_o, \pi_o \right\rangle$ is the one-nucleon-one-meson state vector obtained by applying the operator a^* to the vector $\left| N_o \right\rangle$, and where the dot product in the second term involves a summation in b-space as well as f-space. Here essential use has been made of the linearity of the interaction (10.14b) in the meson field, which restricts the nonvanishing off-diagonal matrix elements of the operator $E - H \pm i\epsilon$ to those which connect states differing by <u>one</u> in the number of mesons present, the values of these elements being given by $-g$ times the elements of the simple vertex operator. One may now write

$$S_\pm(E) = \frac{\underset{\sim}{1}_f}{E - M_o - \Sigma_\pm(E) \pm i\epsilon} = \left[\underset{\sim}{1}_f - S_{o\pm}(E) \cdot \Sigma_\pm(E) \right]^{-1} \cdot S_{o\pm}(E) \quad , \tag{10.27}$$

where

$$\Sigma_\pm(E) = g^2 V_\pm(E) \cdot S_\pm(E - \underset{\sim}{\omega}) \cdot V_o^* \quad , \tag{10.28a}$$

$$V_\pm(E) = g^{-1} \left[S_\pm(E) \right]^{-1} \cdot \left\langle N_o \middle| G_\pm(E) \middle| N_o, \pi_o \right\rangle \cdot \left[S_\pm(E - \underset{\sim}{\omega}) \right]^{-1} . \tag{10.29}$$

Interchange of the order of the factors $G_\pm(E)$ and $(E - H \pm i\epsilon)$ in (10.26) also leads to the same result, but with

$$\Sigma_\pm(E) = g^2 V_o \cdot S_\pm(E - \underset{\sim}{\omega}) \cdot V_\mp(E)^* \quad . \tag{10.28b}$$

It is evident that $S_{o\pm}(E)$, $S_{\pm}(E)$ and $\Sigma_{\pm}(E)$ satisfy relations of the form (7.12) under Hermitian conjugation.

Diagrams

At first sight Eqs. (10.27 to 29) look somewhat unhelpful; $\Sigma_{\pm}(E)$ seems to be a more complicated function than $S_{\pm}(E)$ itself, involving, as it does, both $S_{\pm}(E)$ and the matrix element $\langle N_o | G_{\pm}(E) | N_o, \pi_o \rangle$. However, these equations can be given simple pictorial meanings. Consider first the procedure of evaluating $S_{\pm}(E)$ by a straightforward binomial expansion of Eq. (2.16) and use of (10.14). The expansion will consist of an infinite number of terms, but it is not difficult to see that each term will correspond uniquely to one of the possible ways of putting together the three basic pictorial components illustrated in Fig. 10, each component being used repeatedly any number of times but in such a way that the resulting diagram consists of a single solid vertical line plus any number of emergent and then reentrant dotted lines. The dotted lines are allowed to cross each other, and the order in which the vertices (Fig. 10a, b) occur along the solid line and the manner in which they are paired off is significant. The sole restriction is that only one of the bare-solid-line components (Fig. 10c) is allowed between each pair of vertices, and that the diagram must have just one of these components at the top and one at the bottom.

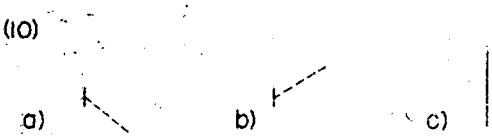
The value of a given term can be read off directly from its corresponding diagram. Each vertex contributes a simple vertex operator multiplied by the coupling constant, each solid line component contributes an unmodified nucleon propagation function, and all these contributions are multiplied together from left to right in the order in which their corresponding components occur from top to bottom in the diagram. A given diagram will

contain as many gV_o-vertices (Fig. 10a) as gV_o^*-vertices (Fig. 10b). The energy value at which a given $S_{o\pm}$ is evaluated will depend on the number of dotted lines intersected by a horizontal line passing through the associated solid line component. The solid line is referred to as a bare nucleon line, the dotted lines are called meson lines, and the whole diagram may be regarded as portraying a process of virtual emission and reabsorption of mesons. The arguments of the unmodified nucleon propagation functions keep a tally of the amount of energy involved in these virtual processes, so that a given S_o will be evaluated not at E but at E minus the sum of the energies of the mesons whose lines are intersected by the horizontal line in question.

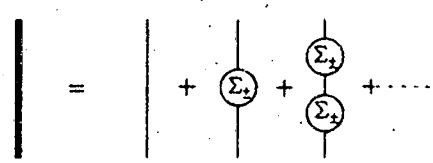
Since each diagram has a definite value associated with it, one may speak of "adding diagrams," meaning that one is adding the corresponding values. The diagrams corresponding to the terms of the expansion of $S_\pm(E)$ may be called real nucleon diagrams. Their sum, i.e. $S_\pm(E)$, will be denoted by a heavy solid line called a real nucleon line. A real nucleon diagram is said to be irreducible if it cannot be separated into two (or more) parts connected only by a single bare nucleon line and no meson lines. If the bare nucleon lines are removed from the top and bottom of an irreducible real nucleon diagram, the result is called a self-energy diagram. The sum of all self-energy diagrams will be denoted by a circle enclosing the symbol $\Sigma_\pm$. It is easy to see that the value of this sum is just the function $\Sigma_\pm(E)$, which will therefore be called the self-energy function; for a real nucleon line may evidently be constructed by the iterative process indicated in Fig. 11, which is just a pictorialization of the binomial expansion of Eq. (10.27).

Next consider the matrix element $\langle N_o | G_\pm(E) | N_o, \pi_o \rangle$. It is not difficult to see that its value may be expressed as the sum of all possible

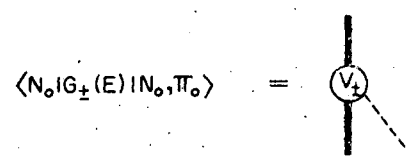
(10)



(11)



(12)



(13)

FIG.10 THE BASIC COMPONENTS OF DIAGRAMS
FIG.11 A PICTORIAL REPRESENTATION OF Eq. (10.27)
FIG.12 A PICTORIAL REPRESENTATION OF Eq. (10.29)
FIG.13 A PICTORIAL REPRESENTATION OF Eqs. (10.26a,b)

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ways of inserting an extra vertex gV_o into all possible real nucleon diagrams. Consider one of these diagrams with the extra vertex inserted. It can generally be split into three parts connected by single bare nucleon lines: a real nucleon diagram at the top, another at the bottom, and an irreducible part containing the extra vertex in the middle. The irreducible part is called a <u>proper vertex diagram</u>. The sum of all proper vertex diagrams will be denoted by a circle enclosing the symbol $V_\pm$, together with an emergent dotted line pointing downward, and will be called a <u>modified vertex</u>. Its reflection in a horizontal line will be denoted by a circle enclosing the symbol $V_\pm^*$, together with an emergent dotted line pointing upward.

Fig. 12 shows the structure of the matrix element $\langle N_o | G_\pm(E) | N_o, \pi_o \rangle$. The modified nucleon propagation function corresponding to the real nucleon line at the bottom of the diagram must evidently be evaluated at $E - \omega$ owing to the presence of the extra meson line. Fig. 12 is therefore a pictorialization of Eq. (10.29), and it is clear the value to be associated with a modified vertex is $gV_\pm(E)$ or $gV_\mp(E)^*$ depending on whether the extra meson line points downward or upward. $V_\pm(E)$ is logically called the <u>modified vertex operator</u>.

There remain Eqs. (10.28a, b) which express further, mainly topological, properties of diagrams. These equations, which are pictured in Fig. 13, state that the sum of all self-energy diagrams is obtainable simply by connecting a modified vertex and a simple vertex by a real nucleon line and a meson line.

Although the practical construction of the modified vertex and nucleon propagation functions and the discussions of renormalization to follow are conveniently carried out in terms of diagrams, objections can be raised against this procedure on the grounds that diagrams are inseparably

connected with a somewhat artificial expansion in powers of the coupling constant, upon which it is unsatisfactory from a purely theoretical point of view to base a theory, particularly since practically nothing is known about the convergence of the expansion or the validity of a defining procedure in terms of analytic continuation. For this reason alternative techniques have been developed which involve only closed variational expressions and avoid use of diagrams altogether. We shall here present one of these techniques which, in addition to having an ability independent of diagrammatic structures to suggest iterative methods of computation, has also the special virtue of rendering the subsequent discussion of renormalization quite straightforward and natural. It is worth emphasizing, however, that we do not attach any special virtue to the avoidance of thinking in terms of diagrams, since the forms of the mathematical structures which will appear have, after all, an unambiguous correlation with the topological properties of special diagrams. Thus, in the later discussion of the S-matrix we shall not hesitate to speak in terms of diagrams when convenient.

A variational technique.*

We begin with a further slight simplification of notation. It will be observed that the total Hamiltonian operator (10.14) is diagonal in the label $\underset{\sim}{r}$. This is a reflection of the immobility of the nucleon in the present example. It will be a convenience for the time being to omit practically all

* For the general ideas contained in the following the author is indebted to Professor Julian Schwinger. (Unpublished lectures given at the Institute for Advanced Study in December, 1954.) To avoid misrepresentation, however, it should be stated that Schwinger bases his variational technique directly on the action principle, while all traces of this approach disappear here.

reference to the nucleon, to replace the symbol $\underset{\sim}{1}_f$ simply by 1, which is to be understood as the unit operator in the space of the matrices T_{iA}, to regard V_o and V_o^* as matrices in this space (thereby ignoring their $\underset{\sim}{r}$ dependence), and to replace the symbols $|N_o\rangle$ and $|N_o, \pi_o\rangle$ by $|0\rangle$ and $|1\rangle$ respectively, the numbers 0 and 1 indicating the number of mesons present in the states in question.

We next introduce the differential operator

$$t = -i\partial/\partial E \,, \tag{10.30}$$

satisfying

$$[E, t] = i \,. \tag{10.31}$$

This operator, which has the effect of producing displacements in energy, will be used in such a way as automatically to accomplish the equivalent of the tally kept by the bare nucleon propagation functions on the meson energies involved in the expansion of $S_\pm(E)$. Since $a^*\cdot\underset{\sim}{\omega}\cdot a\,|0\rangle = 0$, we may write

$$S_\pm = \langle 0|(E - H \pm i\epsilon)^{-1}|0\rangle = \langle 0|e^{ia^*\cdot\underset{\sim}{\omega}\cdot at}(E - H \pm i\epsilon)^{-1} e^{-ia^*\cdot\underset{\sim}{\omega}\cdot at}|0\rangle$$

$$= \langle 0|\left[E - M_o - g(V_o\cdot e^{-i\underset{\sim}{\omega}t}\cdot a + a^*\cdot e^{i\underset{\sim}{\omega}t}\cdot V_o^*) \pm i\epsilon\right]^{-1}|0\rangle \,. \tag{10.32}$$

Here $S_\pm$ is to be regarded as an operator in the vector space of E and t, and hence the argument E is omitted.

It will now be convenient to generalize the definition of the modified nucleon propagation function by replacing the operators a and a^* in (10.32) respectively by $a + \alpha$ and $a^* + \alpha^*$, where α is a variable vector in $\mathfrak{b}$-space whose components $\alpha_{A,\underset{\sim}{p}}$ are ordinary complex numbers. We introduce for brevity the symbols

$$\mathcal{F}_{\pm} = E - M_o - g\left[V_o \cdot e^{-i\underset{\sim}{\omega} t} \cdot (a + \alpha) + (a^* + \alpha^*) \cdot e^{i\underset{\sim}{\omega} t} \cdot V_o^*\right] \pm i\epsilon \ , \tag{10.33}$$

$$\mathcal{G}_{\pm} = \mathcal{F}_{\pm}^{-1} \tag{10.34}$$

so that

$$S_{\pm} = \langle 0 | \mathcal{G}_{\pm} | 0 \rangle \ . \tag{10.35}$$

It is not difficult to show, though unnecessary for our purposes, that $S_{\pm}$, when defined in this way, represents the modified nucleon propagation function when an external meson field

$$\phi_A^{ext}(\underset{\sim}{r}, t) = \sum_{\underset{\sim}{p}} (2\omega L^3)^{-\frac{1}{2}} (\alpha_{A,\underset{\sim}{p}} e^{i(\underset{\sim}{p} \cdot \underset{\sim}{r} - \omega t)} + \alpha_{A,\underset{\sim}{p}}^* e^{-i(\underset{\sim}{p} \cdot \underset{\sim}{r} - \omega t)}) \tag{10.36}$$

is present in addition to the quantized field ϕ_A. The purpose of introducing this external field is to exploit the relation

$$\langle 0 | \mathcal{X} | 1 \rangle = \langle 0 | [\mathcal{X}, a^*] | 0 \rangle = \partial \langle 0 | \mathcal{X} | 0 \rangle / \partial \alpha \ , \tag{10.37}$$

where $\mathcal{X}$ is any operator which, like $\mathcal{F}_{\pm}$ and $\mathcal{G}_{\pm}$, depends on α only through the combination $a + \alpha$. If $\langle 0 | \mathcal{X} | 0 \rangle$ is a quantity which, for $\alpha = 0$, is representable as the sum of a certain set of diagrams then its differentiation with respect to α has the effect of inserting a simple vertex gV_o in all possible ways into these diagrams, thereby producing the quantity $\langle 0 | \mathcal{X} | 1 \rangle$. Although we have written the right side of Eq. (10.37) as an ordinary derivative, it is to be remembered that the differentiation is really a <u>variational</u> one since α is a vector in an ∞ - dimensional space. The present technique is therefore called a

variational technique.

Eq. (10.29) takes on a very simple expression in variational form. Taking care to employ an exponential $e^{i\omega t}$ in such a way as to account for the energy associated with the extra meson line, one has*

$$V_\pm = g^{-1} S_\pm^{-1} \langle 0 | \mathcal{G}_\pm | 1 \rangle S_\pm^{-1} \cdot e^{i\omega t}$$

$$= -g^{-1} (\partial S_\pm^{-1} / \partial \alpha) \cdot e^{i\omega t} \quad . \tag{10.38}$$

The generalized forms of Eqs. (10.27, 28) are obtained essentially by repeating the procedure of Eq. (10.26). Writing

$$1 = \langle 0 | \mathcal{G}_\pm \mathcal{F}_\pm | 0 \rangle = \langle 0 | \mathcal{G}_\pm | 0 \rangle \langle 0 | \mathcal{F}_\pm | 0 \rangle + \langle 0 | \mathcal{G}_\pm | 1 \rangle \cdot \langle 1 | \mathcal{F}_\pm | 0 \rangle \tag{10.39}$$

and making use of (10.33), (10.35) and (10.38), one gets

$$S_\pm = \left[E - M_o - g(V_o \cdot e^{-i\omega t} \cdot \alpha + \alpha^* \cdot e^{i\omega t} \cdot V_o^*) - \Sigma_\pm \pm i\epsilon \right]^{-1} \tag{10.40}$$

with

$$\Sigma_\pm = g^2 V_\pm \cdot e^{-i\omega t} S_\pm \cdot e^{i\omega t} \cdot V_o^* \tag{10.41a}$$

$$= g^2 V_o \cdot e^{-i\omega t} \cdot S_\pm e^{i\omega t} \cdot V_\mp^* \quad . \tag{10.41b}$$

An additional equation may be obtained by combining Eqs. (10.38) and (10.40), namely

$$V_\pm \cdot e^{-i\omega t} = V_o \cdot e^{-i\omega t} + g^{-1} \partial \Sigma_\pm / \partial \alpha \quad . \tag{10.42}$$

---

* Here the dots which indicate the scalar product in f-space have been omitted.

This equation has an obvious topological interpretation in terms of diagrams; it states that a modified vertex is obtained by adding a simple vertex to the result of inserting a simple vertex in all possible ways into the sum of all self-energy diagrams.

In the discussion of renormalization a certain goal will become apparent, namely, to rewrite all mathematical expressions in terms of the modified quantities $S_\pm$ and $V_\pm$. In particular, it will be desirable to remove the hybrid character of Eqs. (10.41a, b) in which both the modified and unmodified vertex operators appear together. This can be accomplished by the following theorem:

$$\begin{aligned}
\langle 0 | \mathcal{F}_\pm \mathcal{X} | 0 \rangle &= \langle 0 | \mathcal{F}_\pm | 0 \rangle \langle 0 | \mathcal{X} | 0 \rangle + \langle 0 | \mathcal{F}_\pm | 1 \rangle \cdot \langle 1 | \mathcal{X} | 0 \rangle \\
&= \langle 0 | \mathcal{F}_\pm | 0 \rangle S_\pm S_\pm^{-1} \langle 0 | \mathcal{X} | 0 \rangle - gV_0 \cdot e^{-i\omega t} \cdot \partial \langle 0 | \mathcal{X} | 0 \rangle / \partial \alpha^* \\
&= \left[(1 - \langle 0 | \mathcal{F}_\pm | 1 \rangle \cdot \langle 1 | \mathcal{G}_\pm | 0 \rangle) S_\pm^{-1} - gV_0 \cdot e^{-i\omega t} \cdot \partial / \partial \alpha^* \right] \langle 0 | \mathcal{X} | 0 \rangle \\
&= (1 - gV_0 \cdot e^{-i\omega t} \cdot S_\pm \partial / \partial \alpha^*)(S_\pm^{-1} \langle 0 | \mathcal{X} | 0 \rangle) .
\end{aligned} \tag{10.43}$$

If one now applies this theorem to the result of taking the variational derivative of the Hermitian adjoint of Eq. (10.39), and uses (10.38), one gets

$$\begin{aligned}
0 &= \left\langle 0 \left| \frac{\partial \mathcal{F}_\pm}{\partial \alpha} \mathcal{G}_\pm \right| 0 \right\rangle + \left\langle 0 \left| \mathcal{F}_\pm \frac{\partial \mathcal{G}_\pm}{\partial \alpha} \right| 0 \right\rangle \\
&= - gV_0 \cdot e^{-i\omega t} S_\pm + g(1 - gV_0 \cdot e^{-i\omega t} \cdot S_\pm \partial / \partial \alpha^*)(V_\pm \cdot e^{-i\omega t} S_\pm) ,
\end{aligned} \tag{10.44}$$

and hence

$$V_o \cdot e^{-i\underset{\sim}{\omega} t} S_\pm = V_\pm \cdot e^{-i\underset{\sim}{\omega} t} S_\pm \cdot \left[\underset{\sim}{1}_b + g \frac{\partial}{\partial \alpha^*} (V_\pm \cdot e^{-i\underset{\sim}{\omega} t} S_\pm) \right]^{-1} , \tag{10.45}$$

which allows one to write

$$\Sigma_\pm = g^2 V_\pm \cdot e^{-i\underset{\sim}{\omega} t} S_\pm \cdot \left[1_b + g \frac{\partial}{\partial \alpha^*} (V_\pm \cdot e^{-i\underset{\sim}{\omega} t} S_\pm) \right]^{-1} \cdot e^{i\underset{\sim}{\omega} t} \cdot V_\mp^* \tag{10.46a}$$

$$= g^2 V_\pm \cdot e^{-i\underset{\sim}{\omega} t} \cdot \left[\underset{\sim}{1}_b + g \left\{ \frac{\partial}{\partial \alpha} (S_\pm e^{i\underset{\sim}{\omega} t} \cdot V_\mp^*) \right\}^T \right]^{-1} S_\pm \cdot e^{i\underset{\sim}{\omega} t} \cdot V_\mp^* , \tag{10.46b}$$

where the superscript T in the second form denotes the transpose in b-space. In Eqs. (10.46a, b) only the modified quantities appear.*

Symmetric theories.

The discussion will now be restricted to field theories for which the simple vertex operator satisfies the conditions

$$\text{Perm} \left[\sum f(p_1, p_2, \ldots) \prod_i V_{oA_i, \underset{\sim}{p}_i} V_{oA_i, \underset{\sim}{p}_i}^* \right] = \text{multiple of unit operator}, \tag{10.47}$$

$$\text{Perm} \left[V_o \sum f(p_1, p_2 \ldots) \prod_i V_{oA_i, \underset{\sim}{p}_i} V_{oA_i, \underset{\sim}{p}_i}^* \right] = \text{multiple of } V_o , \tag{10.48}$$

where

$$V_{oA, \underset{\sim}{p}} = b_{A, \underset{\sim}{p}} \cdot V_o . \tag{10.49}$$

---

* It is interesting to note that Eq. (10.44) may also be solved in the form

$$V_\pm \cdot e^{-i\underset{\sim}{\omega} t} S_\pm = (1 - g V_o \cdot e^{-i\underset{\sim}{\omega} t} \cdot S_\pm \partial / \partial \alpha^*)^{-1} (V_o \cdot e^{-i\underset{\sim}{\omega} t} S_\pm)$$

which enables one to express the self-energy operator in terms of simple vertices only:

$$\Sigma_\pm = g^2 (1 - g V_o \cdot e^{-i\underset{\sim}{\omega} t} \cdot S_\pm \partial / \partial \alpha^*)^{-1} (V_o \cdot e^{-i\underset{\sim}{\omega} t} S_\pm \cdot e^{i\underset{\sim}{\omega} t} \cdot V_o^*) .$$

The summation in (10.47) and (10.48) is to be taken over all the indices $A_i, \underset{\sim}{p}_i$, the symbol "Perm" denotes an arbitrary permutation of the matrices T_{iA} which are contained in the V_o's, and $f(p_1, p_2 \ldots)$ is an arbitrary function of the absolute values of the $\underset{\sim}{p}$'s. When these conditions are satisfied it is not difficult to see (for example, by referring to diagrams) that each internal nucleon state μ plays a role in the meson-nucleon interaction which is symmetric with respect to the roles played by all the others. The theory is therefore said to be <u>symmetric</u>.

The conditions (10.47, 48) are, in practice, not excessively restrictive. All field theories which have been seriously considered, involving only two basic field structures such as Ψ and $\underline{a}$, are without exception symmetric.* In a symmetric theory the perturbation removes no degeneracy. The mass M of a real nucleon, like the mass M_o of the bare nucleon, is the same for all internal states μ. When the external meson field vanishes ($\alpha = 0$), the self-energy operator $\Sigma_\pm$ becomes an ordinary function of E, times the unit operator. Moreover, the modified vertex operator $V_\pm$ becomes an ordinary function of two commuting variables, E and the energy $\underset{\sim}{\omega}$ of the associated meson, times the simple vertex operator V_o. It is sometimes convenient to indicate this explicitly by writing

$$\left(V_\pm\right)_{\alpha=0} = V_o \cdot \Gamma_\pm(E, E - \underset{\sim}{\omega}) , \tag{10.50}$$

$$\left(V_\mp^*\right)_{\alpha=0} = \Gamma_\pm(E - \underset{\sim}{\omega}, E) \cdot V_o^* , \tag{10.51}$$

$$\Gamma_\pm(E, E - \underset{\sim}{\omega})^* = \Gamma_\mp(E - \underset{\sim}{\omega}, E) . \tag{10.52}$$

---

* The introduction of a third field (e.g. the electromagnetic field) can, however, lead to asymmetries.

The structure of the modified nucleon propagation function.

Before proceeding to the renormalization problem let us pause to consider, on physical grounds, what the form of the modified nucleon propagation function should be when the external meson field vanishes. It is useful to make an expansion in terms of the eigenvectors $|\alpha'\rangle$ of the total Hamiltonian operator: [104]

$$S_{\pm}(E) = \langle N_0 | G_{\pm}(E) | N_0 \rangle = \sum_{\kappa} A(\kappa)(E - \kappa \pm i\epsilon)^{-1} \tag{10.53}$$

where

$$A(\kappa) = \sum{}' \langle N_0 | \alpha' \rangle \, \delta_{\kappa E'} \, \langle \alpha' | N_0 \rangle \quad , \tag{10.54}$$

the κ and E' being the eigenvalues of H. The coefficients $A(\kappa)$ are Hermitian dyadics in f-space having positive eigenvalues and satisfying the relations

$$\sum_{\kappa} A(\kappa) = \underset{\sim}{1}_f \quad , \tag{10.55}$$

$$\sum_{\kappa} \kappa A(\kappa) = \langle N_0 | H | N_0 \rangle = M_0 \underset{\sim}{1}_f \quad . \tag{10.56}$$

Since pair creation is prohibited in the present example, only those states $|\alpha'\rangle$ in which exactly one nucleon is present are involved in the expansion (10.54). Of these states a certain set will correspond to the lowest eigenvalue κ occurring in the sum. In a symmetric theory the members of this degenerate set may be taken as the components $|N\rangle \cdot f_{\mu,\underset{\sim}{r}}$ of the real nucleon state vector $|N\rangle$. The eigenvalue in question is M, the mass of the real nucleon. The corresponding amplitude $A(M)$ is given by

$$A(M) = \langle N_0 | N \rangle \cdot \langle N | N_0 \rangle = Z_2 \underset{\sim}{1}_f \quad , \tag{10.57}$$

where Z_2 <u>is the probability of finding the real nucleon in a bare nucleon state</u>.* If the vector $|N\rangle$ is constructed from the vector $|N_0\rangle$ via Eq. (6.8), Z_2 will be the normalization constant Z' of that equation.

We may now write

$$S_{\pm}(E) = Z_2 \frac{1_f}{E - M \pm i\epsilon} + \sum_{K>M} \frac{A(K)}{E - K \pm i\epsilon} . \tag{10.58}$$

In the renormalization program, to be discussed presently, this expression is multiplied by Z_2^{-1} so that the first term, which predominates in the neighborhood of $E = M$, will have exactly the same form as the bare nucleon propagation function (Eq. (10.25)) but with M_0 replaced by M. The result is called the "renormalized" or "corrected" nucleon propagation function and will be denoted by $S_{c\pm}(E)$.

If the coupling constant g is not too large the energy levels of the one-nucleon eigenstates of H other than $|N\rangle \cdot f_{\mu,\underline{r}}$ will generally come from a continuum. These states correspond to the scattering of various numbers of mesons by a real nucleon. For sufficiently large g, however, it may happen that additional discrete levels exist corresponding to one or more stable <u>nucleon isobars</u>. The masses of these isobars must be less than $M + \mu$, for isobars with greater mass will generally decay with the emission of a meson. It is to be noted that the existence of stable isobars will be reflected in the presence of extra poles on the real axis in the function $S_{\pm}(E)$.

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* The subscript 2 on Z_2 has no special significance and is merely an historical accident. It distinguishes this <u>re</u>-normalization constant from the renormalization constant Z_1 which appears later.

Since the $A(\kappa)$ are positive probabilities Eqs. (10.55, 56) allow one to infer the rigorous inequality

$$M < M_0 . \tag{10.59}$$

That is, the nucleon mass is depressed by the perturbation. Another inequality can also be obtained for the mass M_* of the lightest stable isobar (if any), namely

$$M_* < (1 - Z_2)^{-1} (M_0 - Z_2 M) . \tag{10.60}$$

These results hold only for scalar or pseudoscalr theories without nucleon pair creation, such as are embraced in the present example. For vector meson theories or meson pair theories an additional term (which is divergent when the interaction is local) appears on the right hand side of Eq. (10.56).

Renormalization

From the results of experiment we know the value of M, the real nucleon mass, but not the bare mass M_0. It is therefore quite fortunate that the perturbation formalism can be developed in such a way that reference need never be made to M_0. We shall now see how this comes about.

For generality we consider the case in which an external meson field is present, and we write down the first three terms of a double expansion of the self-energy operator $\Sigma_\pm$ in E and α about the points $E = M \mp i\epsilon$ and $\alpha = 0$:

$$\Sigma_\pm = \Delta M - \zeta_2(E - M \pm i\epsilon) + \zeta_1 g(V_0 \cdot e^{-i\omega t} \cdot \alpha + \alpha^* \cdot e^{i\omega t} \cdot V_0^*) + \mathrm{Rem}\, \Sigma_\pm , \tag{10.61}$$

where

$$\Delta M = \left(\Sigma_{\pm}\right)_{\alpha=0,E=M\mp i\epsilon} , \tag{10.62}$$

$$\zeta_2 = -\left(\partial\Sigma_{\pm}/\partial E\right)_{\alpha=0,E=M\mp i\epsilon} , \tag{10.63}$$

$$\zeta_1 = \zeta(\omega_0) , \tag{10.64}$$

$$V_0 \cdot e^{-i\underset{\sim}{\omega} t} \cdot \zeta(\underset{\sim}{\omega}) = g^{-1}\left(\partial\Sigma_{\pm}/\partial\alpha\right)_{\alpha=0,E=M\mp i\epsilon} ,$$

$$\zeta(\underset{\sim}{\omega}) \cdot e^{i\underset{\sim}{\omega} t} \cdot V_0^{*} = g^{-1}\left(\partial\Sigma_{\pm}/\partial\alpha\right)_{\alpha=0,E=M\mp i\epsilon} , \tag{10.65}$$

and where "Rem" denotes the remainder after the constant term and the terms linear in $E - M \pm i\epsilon$ and α have been separated out.

A word of explanation is necessary about the coefficient ζ_1. When $\Sigma_{\pm}$ is differentiated with respect to α, an extra factor $V_0 \cdot e^{-i\underset{\sim}{\omega} t}$, which is not cancelled out by another corresponding factor, remains embedded in each term of an expansion of the resulting expression. The simple vertex operator V_0 can, by the symmetry condition (10.48), be taken out in front of each term provided certain numerical factors are inserted to take into account the algebraic effect of all the other <u>paired</u> vertex operators in these terms. However, the result of similarly displacing the factor $e^{-i\underset{\sim}{\omega} t}$ through the various functions of E involved leaves an expression which is dependent on $\underset{\sim}{\omega}$ as well as E, or on $\underset{\sim}{\omega}$ alone when E is set equal to $M \mp i\epsilon$ and α to zero. For definiteness one must evaluate the factor $\zeta(\underset{\sim}{\omega})$ multiplying $V_0 \cdot e^{-i\underset{\sim}{\omega} t}$ at some fixed meson energy ω_0, as in Eq. (10.64). <u>The choice of</u> ω_0 <u>is completely arbitrary</u>, but once it has been made a term of the form

$$g\left\{V_o \cdot e^{-i\underset{\sim}{\omega}t} \cdot \left[\zeta(\underset{\sim}{\omega}) - \zeta_1\right] \cdot \alpha + \alpha^* \cdot \left[\zeta(\underset{\sim}{\omega}) - \zeta_1\right] \cdot e^{i\underset{\sim}{\omega}t} \cdot V_o^*\right\} \tag{10.66}$$

must evidently be absorbed into Rem $\Sigma_\pm$.

It is customary to make the choice

$$\omega_o = 0 \ . \tag{10.67}$$

The effect of this choice may be expressed compactly by writing

$$\zeta_1 V_o = g^{-1}\left(\partial \Sigma_\pm / \partial \alpha\right)_{\alpha = 0, E = M \mp i\epsilon \ , \underset{\sim}{\omega}_{ext} = 0} \ , \tag{10.68}$$

the instructions "$\underset{\sim}{\omega}_{ext} = 0$" indicating that the energy associated with the external meson field is to be set equal to zero.

The assumed reality of the constants ΔM, ζ_2, ζ_1, and their non-dependence on the $\pm$ signs can easily be checked by referring to the values of the various diagrams associated with Eqs. (10.62 - 65). Since E is set equal to $M \mp i\epsilon$ the bare nucleon propagation functions involved are all real, having the form $(M - M_o - \omega)^{-1}$ where $\omega > \mu$. Owing to the inequality (10.59) no problems arise of integrating around poles, and therefore all the integrals involved in evaluating the diagrams are real and independent of the $\pm$ signs.

If expression (10.61) is substituted into (10.40) and comparison is made with Eq. (10.58) for the case $\alpha = 0$ and in the neighborhood of $E = M$, the following identifications are immediate

$$M = M_o + \Delta M \ , \tag{10.69}$$

$$Z_2 = (1 + \zeta_2)^{-1} \ . \tag{10.70}$$

The constant ΔM is evidently to be interpreted as the nucleon <u>self-mass</u>.

The constant ζ_2 is necessarily positive since $Z_2 < 1$.

If one now introduces the quantities

$$Z_1 = (1 + \zeta_1)^{-1} , \tag{10.71}$$

$$g_c = Z_2 Z_1^{-1} g , \tag{10.72}$$

$$S_{c\pm} = Z_2^{-1} S_\pm , \tag{10.73}$$

$$V_{c\pm} = Z_1 V_\pm , \tag{10.74}$$

$$\mathfrak{M}_\pm = M + Z_2 \operatorname{Rem} \Sigma_\pm , \tag{10.75}$$

it is easy to see that one may rewrite Eqs. (10.38), (10.40), (10.42) and (10.46) respectively in the forms

$$V_{c\pm} = - g_c^{-1} (\partial S_{c\pm}^{-1} / \partial \alpha) \cdot e^{i\underset{\sim}{\omega} t} , \tag{10.76}$$

$$S_{c\pm} = \left[E - \mathfrak{M}_\pm - g_c (V_o \cdot e^{-i\underset{\sim}{\omega} t} \cdot \alpha + \alpha^* \cdot e^{i\underset{\sim}{\omega} t} \cdot V_o^*) \pm i\epsilon \right]^{-1} , \tag{10.77}$$

$$V_{c\pm} = V_o + g_c^{-1} (\partial \mathfrak{M}_\pm / \partial \alpha) \cdot e^{i\underset{\sim}{\omega} t} , \tag{10.78}$$

$$\mathfrak{M}_\pm = M + g_c^2 \operatorname{Rem} V_{c\pm} \cdot e^{-i\underset{\sim}{\omega} t} S_{c\pm} \cdot \left[\underset{\sim}{1}_b + g_c \frac{\partial}{\partial \alpha^*} (V_{c\pm} \cdot e^{-i\underset{\sim}{\omega} t} S_{c\pm}) \right]^{-1} \cdot e^{i\underset{\sim}{\omega} t} \cdot V_{c\mp}^* . \tag{10.79}$$

The quantities $S_{c\pm}$ and $V_{c\pm}$ are the <u>renormalized</u> forms of the modified nucleon propagation function and modified vertex operator respectively. For $\alpha = 0$ and $\underset{\sim}{\omega}_{ext} = 0$ they have the property of reducing essentially to the corresponding unmodified quantities $S_{o\pm}$ (with M_o replaced by M) and V_o in the neighborhood of $E = M$. The quantity $\mathfrak{M}_\pm$ is the so-called <u>mass-operator</u>, which contains within it a description of all the complicated

virtual processes which go to make up the modified nucleon propagation function. In the neighborhood of $E = M$, with $\alpha = 0$, it is equal simply to the real nucleon mass.

The constant g_c is called the renormalized coupling constant. We shall see later how its value may be experimentally determined. For the present we simply note the remarkable fact that its introduction into the formalism allows the various renormalized modified functions to be calculated solely in terms of the experimentally observed constants. Eqs. (10.77 - 79) form together a closed system of equations in terms of which this calculation can be carried out. The physically unobservable constants ΔM, Z_2, Z_1 never appear. By using the variational technique which led to these equations, therefore, one may be said to have developed a pre-renormalized theory. We may of course, at any time we please, evaluate ΔM, Z_2 and Z_1 (at least approximately) in terms of M, g_c, μ, the T_{iA} and the nucleon structure functions $\rho_i(\underset{\sim}{r})$ simply by examining the terms in Eq. (10.79) which are discarded by the symbol "Rem," and thereby determine what the "bare" quantities M_0 and g actually were in the original Hamiltonian operator. But such an evaluation will have theoretical interest only.*

Eqs. (10.77 - 79), being nonlinear variational integro-differential equations, generally cannot be solved in anything even approximating closed form. Recourse must be had to iterative methods of computation. For example,

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* For local interactions, in which the functions $\rho_i(\underset{\sim}{r})$ reduce to the delta function (or its derivatives), the self-mass ΔM is generally divergent, while Z_1 and Z_2 may vanish. In theories which permit pair creation additional renormalization constants come into the picture. The one which is necessary in order to renormalize the modified meson propagation function is generally called Z_3. In the present example $Z_3 = 1$.

One may begin by setting $\mathfrak{M}_{\pm} = M$ and $V_{c\pm} = V_o$ and then calculate cyclically expressions (10.77), (10.79) and (10.78) in that order. No analysis in terms of diagrams is ever necessary by this procedure, but the resulting expressions rapidly become excessively complicated. Moreover, the bracketed inverse in (10.79) must generally be expanded, and it is never practical to retain more than a term or two. For systems of the type we are considering Chew (reference [92]) has used a purely integral iterative technique in which the effect of the variational differentiations is analyzed in terms of infinite families of diagrams, the families becoming more all inclusive the higher the level of approximation. Nothing is known about the convergence of any of these iterative techniques nor about the accuracy of any given level of approximation when g_c is large.

The S-matrix.

The same mathematical structures appear in the expressions for the matrix elements of the scattering operator as have appeared in the discussion of the nucleon propagation function. In particular the value of a given matrix element can be expressed as the sum of values associated with certain diagrams. We shall now investigate some of the characteristics of these evaluations.

We first deal with the operator $\mathcal{R}_{\pm}$ of Eq. (7.19). In order to construct this operator we must redefine the unperturbed Hamiltonian and the perturbation operator in the manner of Eqs. (6.4 - 6). Since the

one-nucleon level shift is ΔM, the operator ΔH_o is to be taken as*

$$\Delta H_o = \Delta M \Psi^* \cdot \Psi . \tag{10.80}$$

Let us suppose that this redefinition has already been carried out.

From Eqs. (2.15) and (7.3) we have

$$G_{o\pm}(E)\mathcal{R}_\pm(E)\, G_{o\pm}(E) = G_\pm(E) - G_{o\pm}(E) , \tag{10.81}$$

where now $\mathcal{R}_\pm(E')|\alpha_o'\rangle = \mathcal{R}_\pm |\alpha_o'\rangle$ and $G_{o\pm}(E) = (E - \mathcal{H}_o \pm i\epsilon)^{-1}$. Taking the expectation value of this expression in the bare nucleon state $|N_o\rangle$ we get

$$(E - M \pm i\epsilon)^{-2} \langle N_o | \mathcal{R}_\pm(E) | N_o \rangle = S_\pm(E) - (E - M \pm i\epsilon)^{-1} \underset{\sim}{1}_f . \tag{10.82}$$

In virtue of (10.58) this implies, in the neighborhood of $E = M$,

$$\langle N_o | \mathcal{R}_\pm(E) | N_o \rangle = (Z_2 - 1)(E - M \pm i\epsilon)\, \underset{\sim}{1}_f , \tag{10.83}$$

from which we may infer

$$\langle N_o | \mathcal{R}_\pm | N_o \rangle = \langle N_o | \mathcal{R}_\pm(M) | N_o \rangle = \mp i\epsilon (1 - Z_2)\, \underset{\sim}{1}_f , \tag{10.84}$$

$$\langle N_o | \left[\partial \mathcal{R}_\pm(E)/\partial E\right]_{E=M} | N_o \rangle = (Z_2 - 1)\, \underset{\sim}{1}_f . \tag{10.85}$$

---

* In the present example this choice is actually correct only for processes involving a single nucleon. If N nucleons are present expression (10.80) has the value $N\Delta M$, but to this must be added the nucleon interaction energy. Scattering by such an <u>array</u> of N fixed nucleons in the present example would correspond to the scattering by a <u>bound</u> system of N nucleons in those theories in which the nucleons are permitted to move.

Substitution of (10.84) into (7.25) leads again, via (7.22), to the identity of Z_2 amd Z' for the one-nucleon-no-meson state.

When mesons are present in addition to the nucleon we shall see that the renormalization constant is still Z_2. This is because the intrinsic properties of the mesons are unaffected by the perturbation in the present example. For definiteness we shall restrict ourselves to the scattering of a single meson by a single nucleon, with no accompanying meson production (e.g. low energy meson-nucleon scattering). That is, we shall investigate the matrix element $\langle N_0, \pi_0 | \mathcal{R}_\pm | N_0, \pi_0 \rangle$.

The diagrams which contribute to this matrix element can be divided into <u>classes</u> which can be put into one-to-one correspondence with the members of a certain set of simple scattering diagrams (constructed out of bare nucleon lines and simple vertices) called <u>irreducible</u>. An irreducible scattering diagram is one which contains no self-energy diagrams nor proper vertex diagrams other than simple vertices in any of its parts. If, in a given irreducible scattering diagram, all the bare nucleon lines are replaced by real nucleon lines and all the simple vertices are replaced by modified vertices, the result is equal to the sum of all the diagrams in the associated class. If all the irreducible scattering diagrams are modified in this way and the results are added together then every possible scattering diagram is correctly accounted for.

In Fig. 14 are shown a few of the irreducible scattering classes. The real nucleon lines at the top and bottom of the diagrams have barred ends. This is to indicate the fact that scattering diagrams actually begin and end with vertices rather than bare nucleon lines. The value of a barred real nucleon line is $S_{0\pm}^{-1} S_\pm$ or $S_\pm S_{0\pm}^{-1}$ according as it is at the top or bottom of the diagram, or $S_{0\pm}^{-1}(S_\pm - S_{0\pm})S_{0\pm}^{-1}$ if it is barred at both ends as in Fig. 14a.

Fig. 14a represents the "singular part" of the operator $\mathcal{R}_{\pm}$, which determines the normalization constant of the meson-nucleon state. In Figs. 14b, c, d the extra meson is attached to the main body of the diagram, being involved in absorption and emission processes. The two vertices of juncture in these cases each contribute a part containing a factor $L^{-3/2}$ (see Eq. (10.16)) which is not absorbed through a momentum integration. These diagrams are therefore of order L^{-3} and contribute to the nonsingular part $\mathcal{R}_{\pm}$ which describes the actual scattering. The meson line in Fig. 14a, on the other hand, is unattached and has the value $\underset{\sim}{1}_b$ indicating that the meson does not change its state. This value multiplies the value of the accompanying nucleon line,* so that the corresponding matrix element is given by**

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* When a single diagram contains two or more unconnected parts the general rule is that the values attached to these parts are to be multiplied (not added) together to obtain the value of the total diagram. In theories in which pair creation is allowed, every diagram can have disjoint accompanying parts; namely those parts in which the vacuum "plays by itself," the so-called vacuum-to-vacuum diagrams. Since these parts are common to all diagrams they are generally ignored, it being assumed that all state vectors have already been multiplied by the vacuum renormalization constant.

** One may wonder at first sight why the operators in Eq. (10.86) are evaluated at $E = M$ rather than at $E = M + \underset{\sim}{\omega}$, $\underset{\sim}{\omega}$ being the meson energy. It is simply necessary to refer back to the original energy denominators $E - \mathcal{H}_0 \pm i\epsilon$. In these denominators E is set equal to $M + \underset{\sim}{\omega}$, but the operator $\mathcal{H}_0$ now must also account for the meson as well as the nucleon, and the net result is as indicated in (10.86).

(14)

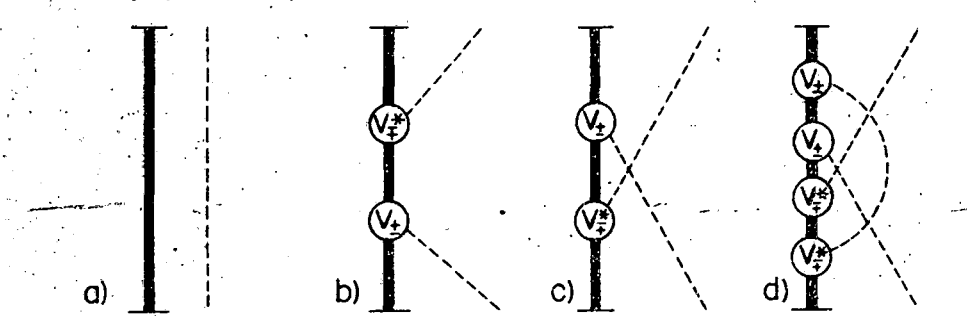

FIG. 14 SOME IRREDUCIBLE SCATTERING DIAGRAMS

MU-10087

$$\left\langle N_o, \pi_o \middle| \text{Sing}\, \mathcal{R}_\pm \middle| N_o, \pi_o \right\rangle = \left[S_{o\pm}^{-1} (S_\pm - S_{o\pm}) S_{o\pm}^{-1} \underset{\sim}{1}_b \right]_{\alpha=0, E=M}$$

$$= \mp i \epsilon (1 - Z_2) \underset{\sim}{1}_f \underset{\sim}{1}_b \quad . \tag{10.86}$$

The normalization constant is therefore again Z_2, the same as for the no-meson state.

In general, when one nucleon is present the renormalized transformation operator $\bar{\mathcal{U}}_c(0, \mp\infty)$ is given (see Eq. (7.34)) by

$$\bar{\mathcal{U}}_c(0, \mp\infty) = Z_2^{-\frac{1}{2}} \bar{\mathcal{U}}(0, \mp\infty) \tag{10.87}$$

no matter how many mesons are present. (If N nucleons were present the factor would be $Z_2^{-N/2}$.) The renormalized (and hence unitary) one-nucleon scattering operator is therefore given by

$$S_c = \bar{\mathcal{U}}_c(\infty, 0) \bar{\mathcal{U}}_c'(0, -\infty) = Z_2^{-1} S \tag{10.88}$$

where S is the operator whose matrix elements are obtained by direct calculation from Eq. (7.40). This operator we may immediately write down. It is, however, now necessary to treat with care the contribution from the singular part of the operator $\mathcal{R}_\pm$, and to include the "derivative term" in (7.40). The value of this latter term follows just as in Eq. (10.85), namely:

$$\left\langle N_o, \pi_o \middle| \left[\text{Sing}\, \partial \mathcal{R}_\pm(E)/\partial E \right]_{E=M+\omega} \middle| N_o, \pi_o \right\rangle = (Z_2 - 1) \underset{\sim}{1}_f \underset{\sim}{1}_b \quad . \tag{10.89}$$

(The nonsingular part does not contribute in the limit $\epsilon \to 0$.) Since Sing $\mathcal{R}_\pm$ is completely diagonal in the $|N_o, \pi_o\rangle$ - representation its matrix elements vary abruptly across the energy shell, and use of the identity (8.27) is forbidden. Instead, the factor $\delta(E'' - E')$ multiplying the

singular contributions in (7.40) must be replaced by $(\pi\epsilon)^{-1}$. Therefore, using (10.86) and (10.89) we have*

$$S = \left[1 - 2\,i\epsilon^{-1}(i\epsilon - \tfrac{1}{2}\,i\epsilon)(Z_2 - 1)\right]\underset{\sim}{1}_f\,\underset{\sim}{1}_b - i\,\underset{\sim}{R}_+$$

$$= Z_2\,\underset{\sim}{1}_f\,\underset{\sim}{1}_b - i\,\underset{\sim}{R}_+ \tag{10.90}$$

where $\underset{\sim}{R}_\pm$ is the operator obtained by taking the matrix elements of the nonsingular part $R_\pm$ on the energy shell.

The decomposition of $\underset{\sim}{R}_\pm$ into terms corresponding to the various irreducible classes of scattering diagrams is as follows

$$\underset{\sim}{R}_\pm = T\,g^2\left[S_{o\pm}^{-1}\,S_\pm\left\{e^{i\underset{\sim}{\omega}t}\cdot V_\mp^*\,S_\pm\,V_\pm\cdot e^{-i\underset{\sim}{\omega}t}\right.\right.$$

$$+ (V_\pm\cdot e^{-i\underset{\sim}{\omega}t}\,S_\pm\,e^{i\underset{\sim}{\omega}t}\cdot V_\mp^*)^T\cdot\left[\underset{\sim}{1}_b - g^2\,S_\pm(V_\pm\cdot e^{-i\underset{\sim}{\omega}t}\,S_\pm\,e^{i\underset{\sim}{\omega}t}\cdot V_\mp^*)^T\right]^{-1}$$

$$\left.\left. + \cdots\right\}\,S_\pm\,S_{o\pm}^{-1}\,\underset{\sim}{1}_f\right]_{\alpha=0,\ \omega_f=\omega_i,\ E=M} \tag{10.91}$$

Here T is the constant of Eq. (8.27), and the notation "$\omega_f = \omega_i$" indicates that the initial and final meson energies are to be taken the same. The first term inside the curly brackets in (10.91) corresponds to Fig. 14b. The second term corresponds to Fig. 14c <u>plus</u> all the diagrams obtainable from it by iteration. (The first term is not similarly iterated since the iterated forms of Fig. 14b lead to redundancies.) The unwritten terms, corresponding to the remaining irreducible classes beginning with Fig. 14d and its iterates, are infinite in number but of higher order in g^2.

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* Here we use the symbols S and $\underset{\sim}{R}_\pm$ to denote what strictly speaking should be denoted by $\langle N_o, \pi_o | S | N_o, \pi_o\rangle$ and $\langle N_o, \pi_o | \underset{\sim}{R}_\pm | N_o, \pi_o\rangle$.

Since

$$\left(S_{o\pm}^{-1} S_{\pm}\right)_{\alpha=0,\ E=M} = \left(S_{\pm} S_{o\pm}^{-1}\right)_{\alpha=0,\ E=M} = Z_2 \tag{10.92}$$

one obtains, using Eqs. (10.72 - 74), (10.88) and (10.90),

$$S_c = \underset{\sim}{1}_f \underset{\sim}{1}_b - i \underset{\sim}{R}_{c+} \tag{10.93}$$

where

$$\begin{aligned}
\underset{\sim}{R}_{c\pm} &= Z_2^{-1} \underset{\sim}{R}_{\pm} \\
&= T g_c^2 \underset{\sim}{1}_f \Big\{ e^{i\underset{\sim}{\omega} t} \cdot V_{c\mp}^{*} S_{c\pm} V_{c\pm} \cdot e^{-i\underset{\sim}{\omega} t} \\
&\quad + (V_{c\pm} \cdot e^{-i\underset{\sim}{\omega} t} S_{c\pm} e^{i\underset{\sim}{\omega} t} \cdot V_{c\mp}^{*})^T \\
&\qquad \cdot \left[\underset{\sim}{1}_b - g_c^2 S_{c\pm} (V_{c\pm} \cdot e^{-i\underset{\sim}{\omega} t} S_{c\pm} e^{i\underset{\sim}{\omega} t} \cdot V_{c\mp}^{*})^T\right]^{-1} \\
&\quad + \cdots \Big\}_{\alpha=0,\ \omega_f = \omega_i,\ E=M}
\end{aligned} \tag{10.94}$$

<u>The renormalized unitary</u> S-<u>matrix may therefore be computed solely in terms of the renormalized coupling constant</u> g_c <u>and the renormalized vertex and propagation functions</u>. The same result holds for scattering in which any number of nucleons and mesons is involved.

<u>The reactance operator.</u>

The renormalization theory of the reactance operator is very similar to that of the S-matrix. We shall first give an outline of the main ideas and then verify that they fit properly into the framework of the theory given in Section 7.

Essentially what one does in dealing with the reactance operator is to follow the same procedures as have already been introduced in the preceding discussion, omitting, however, the imaginary terms $\pm i\epsilon$ wherever they appear and evaluating all integrals in the sense of the principal value. Thus one works with a bare nucleon propagation function of the form

$$S_o(E) = \frac{\underset{\sim}{1}_f}{E - M_o} \tag{10.95}$$

and a real nucleon propagation function of the form

$$S(E) = \frac{\underset{\sim}{1}_f}{E - M_o - \Sigma(E)} \tag{10.96}$$

where

$$\Sigma(E) = g^2\, V(E)\cdot S(E - \underset{\sim}{\omega})\cdot V_o^* = g^2\, V_o\cdot S(E - \underset{\sim}{\omega})\cdot V(E)^* . \tag{10.97}$$

These functions are real everywhere on the real axis and not only for $E < M + \mu$.

The variational technique may again be introduced, permitting the modified vertex operator V to be defined by

$$V\cdot e^{-i\underset{\sim}{\omega}t} = V_o\cdot e^{-i\underset{\sim}{\omega}t} + g^{-1}\, \partial\Sigma/\partial\alpha . \tag{10.98}$$

The renormalization constants are evaluated exactly as before with the use of the obvious modifications of Eqs. (10.61 - 79).

Comparison of Eqs. (7.2) and (7.51) shows that the evaluation of the unrenormalized reactance operator $\underset{\sim}{K}$ may be carried out in terms of diagrams identical with those used to evaluate the operator $\underset{\sim}{R}_\pm$. An important difference appears, however, in the actual expression which one

writes down for $\underset{\sim}{K}$, namely

$$\underset{\sim}{K} = T\, g^2 \left[S_o^{-1}\, S \left\{ e^{i\underset{\sim}{\omega} t} \cdot V^* \, S \, V \cdot e^{-i\underset{\sim}{\omega} t} + \ldots \right\} \underset{\sim}{1}_f \right]_{\alpha=0,\, \omega_f = \omega_i,\, E=M} . \tag{10.99}$$

Here the factor $S\, S_o^{-1}$ which, by analogy with Eq. (10.91), would seem to be required on the right hand side of this expression, is omitted. The reason for this is that the instructions "E = M" now demand an evaluation directly at the pole of the function ~~S~~ in this factor, rather than immediately above or below it. Now, the expression $\left(S\, S_o^{-1}\right)_{\alpha=0,E=M}$ may also be written as $\left[1 - S_o(M) \;\; \Sigma(M)\right]^{-1}$. When $\pm$ signs are inserted this quantity has the value Z_2. However, when they are omitted, as in the present situation, it is to be interpreted as having the value 1, because $\Sigma(M) \equiv 0$ owing to the redefinition (10.80) of the unperturbed Hamiltonian. That is to say, the iterated self-energy diagrams which this quantity evaluates are to be regarded as making no contribution since the nucleon self-energy has been adjusted to zero.

The factor $S_o^{-1}\, S$ on the left is, on the other hand, retained, since it must be treated as a smooth function across the energy shell in order to justify the use of the formal symbol T in front. The value of this factor is evidently to be taken as $\lim_{E \to M} \left[1 - \Sigma(E)\, S_o(E)\right]^{-1} = Z_2$.

The foregoing rules may be described pictorially as the omission of the real nucleon lines at the bottoms of the diagrams in Figs. 14b, c, d, etc. and the omission altogether of Fig. 14a. The omission of Fig. 14a implies that $\underset{\sim}{K}$, unlike $\mathcal{R}_\pm$, has no singular part. Furthermore, since expression (10.99) now has one factor Z_2 less than expression (10.91), the operator

$\underset{\sim}{K}$ appears to be <u>already</u> properly normalized and expressible in the form*

$$\underset{\sim}{K} = T\, g_c^{\,2}\, \underset{\sim}{1}_f \left\{ e^{i\underset{\sim}{\omega} t} \cdot V_c^{\,*}\, S_c\, V_c \cdot e^{-i\underset{\sim}{\omega} t} + \cdots \right\}_{\alpha = 0,\ \omega_f = \omega_i,\ E = M} . \tag{10.100}$$

The correctness of this inference may be readily checked with the aid of Eq. (7.49). One first collects the results of Eqs. (10.83) and (10.86) into the statements

$$\mathcal{R}_\pm = R_\pm \mp i\epsilon(1 - Z_2) , \tag{10.101}$$

$$\underset{\sim}{\mathcal{R}}_\pm = \underset{\sim}{R}_\pm \mp 2\, i(1 - Z_2) , \tag{10.102}$$

and then substitutes into the generalized form of (7.49), getting

$$R_\pm \mp i\epsilon(1 - Z_2) = K(Z_2 \mp \tfrac{1}{2}\, i\, \underset{\sim}{R}_\pm) . \tag{10.103}$$

In taking the matrix elements of this equation on the energy shell one must remember to regard K as smoothly varying across the shell. The singular term on the left must therefore be dropped (which is equivalent to taking the limit $\epsilon \to 0$ before the energy shell operation is carried out) and one gets

$$\underset{\sim}{K} = \frac{\underset{\sim}{R}_{c\pm}}{1 \mp \frac{1}{2}\, i\, \underset{\sim}{R}_{c\pm}} , \tag{10.104}$$

and hence

$$S_c = \frac{1 - \frac{1}{2}\, i\, \underset{\sim}{K}}{1 + \frac{1}{2}\, i\, \underset{\sim}{K}} . \tag{10.105}$$

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* For the more general treatment of the reactance operator in relativistic field theories see reference [32].

A word of caution must be inserted regarding the use of expression (10.100) in formula (10.105) to describe the one-meson scattering problem. If the initial meson kinetic energy is greater than μ so that the production of extra real mesons can take place, then expression (10.100) must be amplified to include matrix elements involving two or more mesons, even though only the one-meson matrix elements of (10.105) may be of interest.

Experimental determination of the renormalized coupling constant.

In order that the renormalization program have a genuine practical utility, there must exist a method whereby the renormalized coupling constant can be measured experimentally in a reasonably direct fashion. We shall first show how it could be measured if a known time independent external meson field could be provided in the laboratory, and then we shall briefly mention the practical difficulties opposing such an arrangement and indicate some possible alternatives.

If the external meson field is $\phi_A^{ext}(\underset{\sim}{r})$ then the average value of the energy of a real nucleon in this field is $M + \langle N | \Delta H | N \rangle$ where

$$\Delta H = g(\Psi^* \cdot V_o \cdot \Psi) \cdot \phi^{ext} , \tag{10.106}$$

$$\phi^{ext} \cdot b_{A,\underset{\sim}{p}} = (2\omega)^{\frac{1}{2}} L^{-3/2} \int \phi_A^{ext}(\underset{\sim}{r})\, e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}}\, d^3\underset{\sim}{r} . \tag{10.107}$$

This average value could be determined by observing the scattering of very slow nucleons as they pass through the field in question. It is only necessary to show that the value of g_c follows immediately from it.

Remembering that

$$|N\rangle = \mathfrak{U}_c(0, \mp\infty) \, | N_o \rangle = Z_2^{-\frac{1}{2}} \left[1 + G_{o\pm}(M) \mathcal{R}_\pm(M) \right] | N_o \rangle , \tag{10.108}$$

one has

$$\left\langle N \,|\, \Delta H \,|\, N \right\rangle = \left\langle N_o \,|\, \bar{\mathcal{U}}_c(\pm\infty,\, 0)\Delta H\, \bar{\mathcal{U}}_c(0, \mp\infty) \,|\, N_o \right\rangle$$

$$= Z_2^{-1}\, g \left[1_f \pm (i\epsilon)^{-1} \left\langle N_o \,|\, \mathcal{R}_\pm(M) \,|\, N_o \right\rangle \right]^2 \cdot V_o \cdot \phi^{ext}$$

$$+ Z_2^{-1}\, g \left\langle N_o \,|\, \mathcal{R}_\pm(M) G_{o\pm}(M) \left(1 - |N_o\rangle \cdot \langle N_o| \right) (\Psi^* \cdot V_o \cdot \Psi) \cdot \phi^{ext} \right.$$

$$\left. G_{o\pm}(M)\, \mathcal{R}_\pm(M) \,|\, N_o \right\rangle . \tag{10.109}$$

By building the appropriate diagrams it is not difficult to see that the second term of (10.109) has the value

$$Z_2^{-1} \left[S_{o\pm}^{-1}\, S_\pm (\partial \Sigma_\pm / \partial \alpha)\, S_\pm\, S_{o\pm}^{-1} \cdot \phi^{ext} \right]_{\alpha=0,\; E=M \mp i\epsilon,\; \omega_{ext}=0}$$

$$= Z_2\, g\, \zeta_1\, V_o \cdot \phi^{ext} . \tag{10.110}$$

(Here the instruction "$\omega_{ext} = 0$" reflects the fact that the external ~~meson~~ meson field, being time independent, feeds no energy into the system.) Using Eqs. (10.71) and (10.84) one therefore gets

$$\left\langle N \,|\, \Delta H \,|\, N \right\rangle = Z_2\, Z_1^{-1}\, g\, V_o \cdot \phi^{ext} = g_c\, V_o \cdot \phi^{ext} . \tag{10.111}$$

Since the structure of the matrices T_{jA}, and hence of V_o, is assumed known, measurement of $\left\langle N \,|\, \Delta H \,|\, N \right\rangle$ for various internal nucleon states affords a direct determination of g_c.

The great difficulty, of course, is that meson fields have extremely short range, owing to the finite meson mass, and therefore cannot be produced on a macroscopic, and hence classical, scale in the laboratory. Never more than a small number of nucleons (e.g. those in a single atomic nucleus) contribute effectively to a given meson field at any point. Therefore the

quantum character of the meson field is always dominant in any physical process in which it takes part, and the calculation of the average value of the field is generally insufficient to solve the corresponding theoretical problem. This is unfortunate, because average values are easy to compute.

As an illustration of the difficulty, consider the average value of the meson field produced by a single real nucleon. This is given by

$$\langle \phi_A(\underset{\sim}{r}) \rangle = \sum_{\underset{\sim}{p}} (2\omega L^3)^{-\frac{1}{2}} \langle N | (a_{A,\underset{\sim}{p}} e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}} + a_{A,\underset{\sim}{p}}^* e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}}) | N \rangle . \tag{10.112}$$

In order to evaluate this expression first observe, using (10.10) and (10.14), that

$$[a, H] = \underset{\sim}{\omega}\cdot a + g \Psi^* \cdot V_o^* \cdot \Psi \quad . \tag{10.113}$$

Therefore, rewriting Eq. (10.108) in the form (6.8), namely

$$| N \rangle = \pm i\epsilon \, Z_2^{-\frac{1}{2}} (M - H \pm i\epsilon)^{-1} | N_o \rangle \quad , \tag{10.114}$$

and remembering that $a | N_o \rangle = 0$, one gets

$$\begin{aligned} a | N \rangle &= \pm i \epsilon \, Z_2^{-\frac{1}{2}} \left[a, (M - H \pm i\epsilon)^{-1} \right] | N_o \rangle \\ &= (M - H \pm i\epsilon)^{-1} (\underset{\sim}{\omega}\cdot a + g \Psi^* \cdot V_o^* \cdot \Psi) | N \rangle \\ &= g(M - \underset{\sim}{\omega} - H \pm i\epsilon)^{-1} \cdot (\Psi^* \cdot V_o^* \cdot \Psi) | N \rangle . \end{aligned} \tag{10.115}$$

Use of (10.111) then yields

$$\langle N | a | N \rangle = - g_c (\underset{\sim}{\omega} \mp i\epsilon)^{-1} \cdot V_o^* . \tag{10.116}$$

The $\mp i\epsilon$ in this expression plays no role in the summation over meson energies and may be ignored. Therefore

$$\langle \phi_A(\underset{\sim}{r}) \rangle = -2\,\mathrm{Re}\, g_c \sum_{\underset{\sim}{p}} (2\omega^3 L^3)^{-\frac{1}{2}} V_{oA,\underset{\sim}{p}}{}^* e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}}$$

$$= -g_c \sum_{j,\mu,\nu,\underset{\sim}{r}'} f_{\mu,\underset{\sim}{r}'} (T_{jA})_{\mu\nu} f_{\nu,\underset{\sim}{r}'} \mathcal{V}_{j,i\underset{\sim}{\nabla}} Y(\underset{\sim}{r} - \underset{\sim}{r}') \tag{10.117}$$

where

$$Y(\underset{\sim}{r}) = L^{-3} \sum_{\underset{\sim}{p}} \omega^{-2} e^{\pm i\underset{\sim}{p}\cdot\underset{\sim}{r}} = (4\pi)^{-1} e^{-\mu r}/r \,, \tag{10.118}$$

If now one were to regard $\langle \phi_A(r) \rangle$ as the external field appearing in (10.107), one would obtain $\phi^{ext} = -2\, g_c\, \underset{\sim}{\omega}^{-1} \cdot V_o{}^*$. If this were used in Eq. (10.111), one would get for the potential energy of interaction between <u>two</u> nucleons, the expression

$$-2\, g_c{}^2\, V_o \cdot \underset{\sim}{\omega}^{-1} \cdot V_o{}^*$$

$$= -g_c{}^2 \sum f_{\mu,\underset{\sim}{r}} (T_{jA})_{\mu\nu} f_{\nu,\underset{\sim}{r}} f_{\mu',\underset{\sim}{r}'} (T_{j'A})_{\mu'\nu'} f_{\nu',\underset{\sim}{r}'} \mathcal{V}_{j,-i\underset{\sim}{\nabla}} \mathcal{V}_{j',i\underset{\sim}{\nabla}} Y(\underset{\sim}{r} - \underset{\sim}{r}'), \tag{10.119}$$

where the summation is to be carried out over all visible indices.* This, however, is only the first term in a series expansion of the exact expression in powers of $g_c{}^2$. If g_c were small this first term could, of course, reasonably be expected to give a fair approximation to the exact expression, so that the interaction potential would be basically classical in spite of the microscopic dimensions involved, and an experimental investigation of

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* The dot products on the left of (10.119) are meant to imply b-space summations only. Therefore the expression is a <u>double</u> dyadic in f-space, which allows for all the possible positions and internal states of both nucleons.

nuclear two-body forces (which immediately suggests itself) would give direct information on the value of g_c. Unfortunately there seems no reason to believe that g_c is small, and therefore the purely quantum effects in the two-body problem must be determined. This general problem is so difficult, however, that no simple exact solution comparable to (10.119) exists with which to correlate observed nuclear binding energies, moments, etc.

The next thing that suggests itself therefore is to investigate the possibilities inherent in the somewhat simpler problems of meson-nucleon scattering and photo-meson production. The results of this investigation have led to the so-called <u>threshold theorems</u>. [95 to 103] The threshold theorem for scattering will now be derived.*

One first obtains the equation involving a^* analogous to (10.115). Using the Hermitian adjoint of Eq. (10.113) and remembering that $a^* \left| N_o \right\rangle = \left| N_o, \pi_o \right\rangle$, one gets

$$a^* \left| N \right\rangle = - g(M + \underset{\sim}{\omega} - H \pm i\epsilon)^{-1} \cdot (\Psi^* \cdot V_o \cdot \Psi) \left| N \right\rangle + \left| N, \pi, \pm \right\rangle \tag{10.120}$$

where

$$\left| N, \pi, \pm \right\rangle = \bar{\mathfrak{U}}_c(0, \mp \infty) \left| N_o, \pi_o \right\rangle = \pm i\epsilon Z_2^{-\frac{1}{2}} (M + \underset{\sim}{\omega} - H \pm i\epsilon)^{-1} \left| N_o, \pi_o \right\rangle . \tag{10.121}$$

Use of the Hermitian adjoint of Eq. (10.120) allows one to write

$$\left\langle N, \pi, \mp \middle| N, \pi, \pm \right\rangle = \left\langle N \middle| \left[a + g(\Psi^* \cdot V_o^* \cdot \Psi) \cdot (M + \underset{\sim}{\omega} - H \pm i\epsilon)^{-1} \right] \middle| N, \pi, \pm \right\rangle$$

$$= \left\langle N, \pi, \pm \middle| N, \pi, \pm \right\rangle + g \left\langle N \middle| (\Psi^* \cdot V_o^* \cdot \Psi) \cdot \left[-(M + \underset{\sim}{\omega} - H \pm i\epsilon)^{-1} \quad (M + \underset{\sim}{\omega} - H \pm i\epsilon)^{-1} \right] \middle| N, \pi, \pm \right\rangle$$

$$\rightarrow \underset{\sim}{1}_f \, \underset{\sim}{1}_b \mp i \, \underset{\sim}{R}_{c\pm} , \tag{10.122}$$

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* The present derivation is essentially due to F. Low, references [93] and [99].

where

$$R_{c\pm} = g\left\langle N \left| \Psi^* \cdot V_o^* \cdot \Psi \right| N, \pi, \pm \right\rangle \quad . \tag{10.123}$$

The operator $\underset{\sim}{R}_{c\pm}$, obtained by taking $R_{c\pm}$ on the energy shell, is obviously identical with the $\underset{\sim}{R}_{c\pm}$ of Eq. (10.94), and hence differs from $\underset{\sim}{R}_{\pm}$ only by the numerical factor Z_2^{-1}. The operator $R_{c\pm}$ itself, when defined by (10.123), is however not a simple multiple of $R_{\pm}$ (the nonsingular part of $\mathcal{R}_{\pm}$) as may be seen by examining the bare nucleon propagation functions in the expansion of (10.123) and noting that, except on the energy shell, they do not keep a proper tally of the meson energies above the vertex introduced by the operator $\Psi^* \cdot V_o^* \cdot \Psi$.

Using both Eqs. (10.115) and (10.120), and remembering that a^* commutes with $\Psi^* \cdot V_o^* \cdot \Psi$, one may reexpress $R_{c\pm}$ in the form

$$\begin{aligned}
R_{c\pm} &= g\left\langle N \left| \Psi^* \cdot V_o^* \cdot \Psi \left[a^* + g(M + \underset{\sim}{\omega} - H \pm i\epsilon)^{-1} \cdot (\Psi^* \cdot V_o \cdot \Psi) \right] \right| N \right\rangle \\
&= g^2 \left\langle N \left| \left\{ \left[(\Psi^* \cdot V_o \cdot \Psi) \cdot (M - \underset{\sim}{\omega} - H)^{-1} \Psi^* \cdot V_o^* \cdot \Psi \right]^T \right.\right. \\
&\qquad \left.\left. + \Psi^* \cdot V_o^* \cdot \Psi (M + \underset{\sim}{\omega} - H \pm i\epsilon)^{-1} \cdot (\Psi^* \cdot V_o \cdot \Psi) \right\} \right| N \right\rangle \\
&= g^2 \sum{}' \left\{ \left[\left\langle N \left| \Psi^* \cdot V_o \cdot \Psi \right| \alpha' \right\rangle \cdot (M - \underset{\sim}{\omega} - E')^{-1} \left\langle \alpha' \left| \Psi^* \cdot V_o^* \cdot \Psi \right| N \right\rangle \right]^T \right. \\
&\qquad \left. + \left\langle N \left| \Psi^* \cdot V_o^* \cdot \Psi \right| \alpha' \right\rangle (M + \underset{\sim}{\omega} - E' \pm i\epsilon)^{-1} \cdot \left\langle \alpha' \left| \Psi^* \cdot V_o \cdot \Psi \right| N \right\rangle \right\}
\end{aligned} \tag{10.124}$$

where the $|\alpha'\rangle$ are the eigenvectors of H. Keeping only the term

$|\alpha'\rangle = |N\rangle$, one has*

$$R_{c\pm} = g_c^2 \left[V_o^* \underset{\sim}{\omega}^{-1} \cdot V_o - (V_o \cdot \underset{\sim}{\omega}^{-1} V_o^*)^T \right] + \cdots \tag{10.125}$$

(The dots indicating dyadic multiplication in f-space have been omitted in this expression.) This result may be substituted directly into Eq. (8.19) to obtain the meson scattering cross section. In this case $v' = p'/\omega'$, and one finds to lowest order in g_c

$$\sigma(\underset{\sim}{\Omega}, A'' | \underset{\sim}{p}', A') = (g_c^2/4\pi)^2 \omega'^{-2} \left| \sum_{i,j} v_{j,\underset{\sim}{\Omega}p'}^* v_{i,\underset{\sim}{p}'} \left[T_{jA''}, T_{iA'} \right] \right|^2 . \tag{10.126}$$

Here a summation is implied over the various possible final states of the nucleon.

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* If the nucleon is located at the origin, then in many theories the V_o and V_o^* in the first term inside the curly brackets of (10.124) may be replaced by V_o^* and V_o respectively, so that if one includes also the terms $|\alpha'\rangle = |N, \pi, \pm\rangle$ one obtains a nonlinear integral equation for $R_{c\pm}$, namely —

$$b_{A'',\underset{\sim}{p}''} \cdot R_{c\pm} \cdot b_{A',\underset{\sim}{p}'} = g_c^2 \omega'^{-1} \left[V_{oA'',\underset{\sim}{p}''}, V_{oA',\underset{\sim}{p}'} \right]$$

$$+ \sum''' \frac{b_{A',\underset{\sim}{p}'} \cdot R_{c\pm} \cdot b_{A''',\underset{\sim}{p}'''} \; b_{A''',\underset{\sim}{p}'''} \cdot R_{c\pm}^* \cdot b_{A'',\underset{\sim}{p}''}}{-\omega' - \omega'''}$$

$$\frac{b_{A'',\underset{\sim}{p}''} \cdot R_{c\pm} \cdot b_{A''',\underset{\sim}{p}'''} \; b_{A''',\underset{\sim}{p}'''} \cdot R_{c\pm}^* \cdot b_{A',\underset{\sim}{p}'}}{\omega' - \omega''' \pm i\epsilon}$$

To shift the nucleon to an arbitrary position $\underset{\sim}{r}$ one simply multiplies this expression by $e^{i(\underset{\sim}{p}' - \underset{\sim}{p}'') \cdot \underset{\sim}{r}}$. If still more terms are included then it is necessary to derive further equations, analogous to (10.115) and (10.120), involving the application of the operators a and a* twice or more to the vector $|N\rangle$, and leading to a series of coupled nonlinear integral equations.

At first sight we seem to be no better off than in the two-body problem, for expression (10.126) is certainly not a good approximation to the exact cross section if g_c is not small. However, if one is willing to assume that the exact expression is a smooth function of ω' in the neighborhood of μ as well as in the nonphysical region between 0 and then one may extrapolate the experimental results backward from the low meson kinetic energy region to $\omega' = 0$, at which point the term (10.125) completely dominates all the other terms in (10.124) so that the cross section formula (10.126) does become exact. Formula (10.126) may contain, of course, a factor depending on $p' = (\omega'^2 - \mu^2)^{\frac{1}{2}}$ and having either a branch point or a zero at $\omega' = \mu$ which prevents a direct extrapolation of the experimental results to $\omega' = 0$. However, the observed cross section may be multiplied by the reciprocal of this factor and then extrapolated. A direct determination of g_c is thereby achieved, provided the assumption of smoothness is valid.*

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* In the pseudovector coupling theory considered by Chew, [92] integration of Eq. (10.126) over all angles and averaging over all initial nucleon states leads to a total cross section $\sigma(\omega') = (4/3\pi)(g_c/\mu)^4 p'^4/\omega'^2$. The renormalized coupling constant is therefore determined by

$$\left(\frac{g_c}{\mu}\right)^4 = \lim_{\omega' \to 0} \frac{3\pi}{4} \frac{\omega'^2}{(\omega'^2 - \mu^2)^2} \sigma_{obs}(\omega') .$$

Here σ_{obs} must refer only to observed P-wave scattering, since S-wave scattering is not described by the pseudovector coupling.

The substance of the threshold theorem is contained in the following statement: <u>The cross section for scattering of a meson of zero energy is given exactly by the lowest order perturbation expression, with</u> g <u>replaced by</u> g_c, (Eq. (10.126)). The statement is rigorously true and depends neither on the masses of the virtual mesons nor on the magnitude of g_c.

<u>Fourier transforms.</u>

The particle propagation functions are frequently introduced through their Fourier transforms, as they then have a more direct connection with the field variables. This connection may be seen by defining

$$S_\pm(t) = (2\pi)^{-1}\int_{-\infty}^{\infty} S_\pm(E)\, e^{-iEt}\, dE \tag{10.127}$$

and making use of Eqs. (1.15), (2.9), (2.13), (10.20) and (10.21), and the fact that $V(0, t) = U(t, 0)$ when the total Hamiltonian operator is time independent. Evidently

$$\begin{aligned} S_\pm(t) &= \left\langle N_o \middle| G_\pm(t, 0) \middle| N_o \right\rangle \rightarrow \mp i\, \theta_\pm(t) \left\langle N_o \middle| U(t,0) \middle| N_o \right\rangle \\ &= \mp i\, \theta_\pm(t) \left\langle \text{vac} \middle| U(0, t)\, \Psi\, U(t, 0) \middle| N_o \right\rangle \\ &= \mp i\, \theta_\pm(t) \left\langle \text{vac} \middle| \underset{\sim}{\Psi}(t) \middle| N_o \right\rangle \end{aligned} \tag{10.128}$$

where $\underset{\sim}{\Psi}(t)$ is the nucleon field variable in the Heisenberg representation.

Expression (10.128) may also be rewritten in the more symmetric form

$$\begin{aligned} S_\pm(t'' - t') &= \mp i\, \theta_\pm(t'' - t') \left\langle N_o \middle| U(t'', t') \middle| N_o \right\rangle \\ &= \mp i\, \theta_\pm(t'' - t') \left\langle \text{vac} \middle| \underset{\sim}{\Psi}(t'')\, \underset{\sim}{\Psi}^*(t') \middle| \text{vac} \right\rangle . \end{aligned} \tag{10.129}$$

Using the fact that $\underset{\sim}{\Psi}(t)\,|\,\mathrm{vac}\rangle = 0$ one may further modify this equation to

$$S_{\pm}(t'' - t') = \mp i \langle \mathrm{vac} | \left[\underset{\sim}{\Psi}(t'') \underset{\sim}{\Psi}^*(t') \right]_{\pm} | \mathrm{vac} \rangle$$

$$= - i\sigma(t'' - t') \langle \mathrm{vac} | \left[\underset{\sim}{\Psi}(t'') \underset{\sim}{\Psi}^*(t') \right]_{\pm} | \mathrm{vac} \rangle \quad . \tag{10.130}$$

Time-ordered expressions like (10.130) have a useful form in the interaction representation. First consider the general expression $\langle \alpha_{\mp}' | \underset{\sim}{F}(t_1)\, \underset{\sim}{G}(t_2) | \alpha_{\pm}' \rangle$ where $\underset{\sim}{F}$ and $\underset{\sim}{G}$ are arbitrary Heisenberg operators and $|\alpha_{\pm}'\rangle$ is an eigenvector of H corresponding to the eigenvector $|\alpha_0'\rangle$ of $\mathcal{H}_0$. Remembering that $\underset{\sim}{F}(t) = \bar{\mathcal{U}}(0, t)\bar{F}(t)\bar{\mathcal{U}}(t, 0)$ one may write this expression in the form

$$\langle \alpha_{\mp}' | \underset{\sim}{F}(t_1)\, \underset{\sim}{G}(t_2) | \alpha_{\pm}' \rangle$$

$$= Z'^{-1} \langle \alpha_0' | \bar{\mathcal{U}}(\pm\infty, t_1)\bar{F}(t_1)\bar{\mathcal{U}}(t_1, t_2)\bar{G}(t_2)\bar{\mathcal{U}}(t_2, \mp\infty) | \alpha_0' \rangle \quad . \tag{10.131}$$

The combination of this result with Eqs. (1.31, 32) evidently gives

$$\langle \alpha_{\mp}' | \left[\underset{\sim}{F}(t_1) \underset{\sim}{G}(t_2) \right]_{\pm} | \alpha_{\pm}' \rangle$$

$$= Z'^{-1} \langle \alpha_0' | \left[\bar{F}(t_1)\, \bar{G}(t_2)\, \exp(\mp i \int_{-\infty}^{\infty} \bar{\mathcal{H}}_1(t)dt) \right]_{\pm} | \alpha_0' \rangle \quad . \tag{10.132}$$

The renormalization constant Z' of the state $|\alpha_{\pm}'\rangle$ may be similarly expressed:

$$Z' = \mathrm{Sing} \langle \alpha_0' | \bar{\mathcal{U}}(\pm\infty, \mp\infty) | \alpha_0' \rangle$$

$$= \mathrm{Sing} \langle \alpha_0' | \left[\exp(\mp i \int_{-\infty}^{\infty} \mathcal{H}_1(t)dt) \right]_{\pm} | \alpha_0' \rangle \quad . \tag{10.133}$$

In the present example $Z' = 1$ for the vacuum state, and therefore

$$S_{\pm}(t'' - t') = -i\sigma(t'' - t') \left\langle \text{vac} \left| \left[\bar{\Psi}(t'')\bar{\Psi}^*(t') \exp(\mp i \int_{-\infty}^{\infty} \bar{\mathcal{H}}_1(t)dt) \right]_{\pm} \right| \text{vac} \right\rangle . \tag{10.134}$$

This equation is also correct in theories which allow pair creation, provided all vacuum-to-vacuum effects are consistently ignored.

In relativistic field theories the traditional development proceeds from expressions of the form (10.134). The nucleon propagation function is, however, then defined by

$$S_{\pm}(\chi'' - \chi') = -i\sigma(t'' - t') \left\langle \text{vac} \left| \left[\underset{\sim}{\psi}(\chi'') \underset{\sim}{\psi}^*(\chi') \right]_{\pm} \right| \text{vac} \right\rangle , \tag{10.135}$$

in which the space and time coordinates are placed on equal footing: $(\chi') = (\underset{\sim}{r}', it')$. In the present example this function reduces to the nonrelativistic form

$$S_{\pm}(\chi'' - \chi') = \delta(\underset{\sim}{r}'' - \underset{\sim}{r}') S_{\pm}(t'' - t') . \tag{10.136}$$

The analogous structure for the mesons, on the other hand, is relativistically covariant. The Fourier transform of the meson propagation function defined by Eq. (10.24) is evidently

$$\mp i \left\langle \text{vac} \left| \left[\underset{\sim}{a}(t'') \underset{\sim}{a}^*(t') \right]_{\pm} \right| \text{vac} \right\rangle = \mp i\, \Theta_{\pm}(t'' - t')\, e^{-i\underset{\sim}{\omega}(t'' - t')} . \tag{10.137}$$

Therefore

$$\begin{aligned} &\mp i \left\langle \text{vac} \left| \left[\underset{\sim}{\varphi}_{A''}(\chi'') \underset{\sim}{\varphi}_{A'}(\chi') \right]_{\pm} \right| \text{vac} \right\rangle \\ &= \mp i \sum_{\underset{\sim}{p}', \underset{\sim}{p}''} (2L^3)^{-1} (\omega'' \omega')^{-\frac{1}{2}} \left\langle \text{vac} \left| \left[(\underset{\sim}{a}_{A'', \underset{\sim}{p}''}(t'') e^{i\underset{\sim}{p}'' \cdot \underset{\sim}{r}''} \right.\right.\right. \\ &\qquad \left.\left.\left. + \underset{\sim}{a}_{A'', \underset{\sim}{p}''}^*(t'') e^{-i\underset{\sim}{p}'' \cdot \underset{\sim}{r}''}) (\underset{\sim}{a}_{A', \underset{\sim}{p}'}(t') e^{i\underset{\sim}{p}' \cdot \underset{\sim}{r}'} + \underset{\sim}{a}_{A', \underset{\sim}{p}'}^*(t') e^{-i\underset{\sim}{p}' \cdot \underset{\sim}{r}'}) \right]_{\pm} \right| \text{vac} \right\rangle \\ &= \delta_{A''A'} \Delta_{\pm}(\chi'' - \chi') \end{aligned} \tag{10.138}$$

where

$$\Delta_{\pm}(x) = \mp i \sum_{\underset{\sim}{p}} (2\omega L^3)^{-1} \left[\theta_{\pm}(t)\, e^{i(\underset{\sim}{p}\cdot\underset{\sim}{r} - \omega t)} + \theta_{\mp}(t)\, e^{-i(\underset{\sim}{p}\cdot\underset{\sim}{r} - \omega t)}\right]$$

$$= -(2\pi)^{-4} \int \underline{(k^2 + \mu^2 \mp i\eta)}^{-1}\, e^{ikx}\, d^4k\,, \qquad (10.139)$$

with

$$(k) = (\underset{\sim}{p},\, i\, p_0)\,, \qquad d^4k = d^3\underset{\sim}{p}\, dp_0\,, \qquad \text{and} \qquad \eta = 2\omega\epsilon\,.$$

Some remarks.

The operator formalism finds probably its richest expression in its application to field theories. Obviously the foregoing discussion can be carried on into many other ramifications of the subject. To take just one example, the concept of the propagation function can be applied not only to a single particle but to any number of simultaneously interacting particles. One simply introduces structures similar to (10.130) but involving arbitrary numbers of operator pairs $\underset{\sim}{\Psi}$, $\underset{\sim}{\Psi}^*$, plus any number of repetitions of the operators $\underset{\sim}{a}$ and $\underset{\sim}{a}^*$. The resulting functions involve separate "emission times" and separate "absorption times" for each particle. If all the emission times are set equal and all the absorption times are set equal, and if the Fourier transform is taken of the result, one obtains essentially the quantities $\langle n, m'' | G_{\pm}(E) | n, m' \rangle$, where $| n, m \rangle$ denotes the state-vector describing n bare nucleons and m bare mesons. Owing to the simple connection (Eq. (10.81)) between the Green's function and the scattering operator, discussion of scattering can be carried out solely in terms of these functions. The many-particle propagation functions also provide the appropriate framework in which to study bound state problems. Moreover, if the various emission and absorption times are left independent, as is especially appropriate in a relativistic theory, they provide a method of

carrying out the renormalization program (in particular the proof that the renormalized S-matrix involves only observable quantities) in a simpler and more natural fashion than that outlined above. Lack of space, however, prevents these applications from being described here. A few of the pertinent references are included in the bibliography at the end of the article.

Another topic about which silence will be maintained is the question of the "renormalizability" of a given theory. This is the question of whether or not the various integrals remaining after renormalization has been performed are all convergent. This question arises only for local theories (infinite cut-off), ~~and the~~ answer to it depends on details of the interaction. Although of practical importance, the subject is highly specialized and has no bearing on the operator formalism.

We shall also say nothing about radii of convergence for the expansions of renormalized matrix elements in powers of g_c, nor about the question of whether or not the expansions might have some meaning even if the radii happen to vanish.

The neutral scalar field.

It is well known that the coupled field problem can be solved exactly if the matrices T_{jA} occurring in the vertex operators commute with one another.* It is of interest to show this within the context of renormalization theory. One must first recall that the functional dependence of the operators $S_\pm$, $\Sigma_\pm$, $V_\pm$ on E and α always occurs through the combination $E - g(V_0 \cdot e^{-i\omega t} \cdot \alpha + \alpha^* \cdot e^{i\omega t} \cdot V_0)$. Therefore, if the vertices commute so

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* G. Wentzel, reference [7]. For other interesting field problems which can be solved exactly see references [108,109,110].

that the numerical factors appearing in various terms, under the operation involved in Eq. (10.65), are all equal to unity, and if the energy associated with the external meson field is set equal to zero, then differentiation with respect to α is essentially equivalent to differentiation with respect to E. This implies, for example (see Eqs. (10.38) and (10.50))

$$\Gamma_{\pm}(E, E) = \partial S_{\pm}^{-1}(E)/\partial E \quad . \tag{10.140}$$

In particular (setting $E = M \mp i\epsilon$)

$$Z_1^{-1} = Z_2^{-1} \tag{10.141}$$

and hence

$$g_c = g \quad . \tag{10.142}$$

Eq. (10.140) can be generalized to include the useful case in which the external meson energy does not vanish. The reasoning is as follows: If the vertices commute then to any function F(E) there corresponds a <u>unique</u> function F of $E - g(V_o \cdot e^{-i\omega t} \cdot \alpha + \alpha^* \cdot e^{i\omega t} \cdot V_o^*)$ from which F(E) can be obtained by setting $\alpha = 0$. One may therefore define the following operation:

$$F_{,\alpha}(E) = \left(\partial F/\partial\alpha\right)_{\alpha=0} \cdot e^{i\omega t} \quad . \tag{10.143}$$

For example:

$$\text{If} \quad F(E) = E \quad \text{then} \quad F_{,\alpha}(E) = -g\, V_o \quad . \tag{10.144}$$

The general result of performing this operation on an arbitrary function of E, which is analytic in some region, may be obtained by induction from (10.144) together with the following tally-keeping rules for the meson energy:

If $F(E) = F_1(E)\, F_2(E)$ then

$$F_{,\alpha}(E) = F_{1,\alpha}(E)\cdot F_2(E - \omega) + F_1(E)\, F_{2,\alpha}(E) \,. \tag{10.145}$$

If $F(E) = G^{-1}(E)$ then

$$F_{,\alpha}(E) = -G^{-1}(E)\, G_{,\alpha}(E)\cdot G^{-1}(E - \omega) \,. \tag{10.146}$$

The functions $S_\pm(E)$, $\Sigma_\pm(E)$, $\Gamma_\pm(E, E - \omega)$ are presumed to have a region of analyticity, and hence these rules apply to them in particular.

Using rules (10.144 - 146) one may easily prove the following theorem:

$$F_{,\alpha}(E) = -g\, V_o \cdot \left[F(E) - F(E - \omega)\right] \cdot \omega^{-1} \,. \tag{10.147}$$

If $F(E) = E$ the theorem is obvious, and the general case follows by induction. Since $V_o \cdot \Gamma_\pm(E, E - \omega) = g^{-1}\, S_\pm^{-1}{}_{,\alpha}(E)$ one may therefore infer

$$\Gamma_\pm(E, E - \omega) = \left[S_\pm^{-1}(E) - S_\pm^{-1}(E - \omega)\right] \cdot \omega^{-1} \,, \tag{10.148}$$

which reduces to (10.140) in the limit $\omega \to 0$. Inserting this result together with Eq. (10.50) into (10.41a) for the case $\alpha = 0$, one obtains the following expression for the self-energy function

$$\Sigma_\pm(E) = g^2\, V_o \cdot \left[S_\pm^{-1}(E) - S_\pm^{-1}(E - \omega)\right] \cdot \omega^{-1} \cdot S_\pm(E - \omega) \cdot V_o^* \,, \tag{10.149}$$

which, when substituted into Eq. (10.27), yields the simple integral equation

$$(E - M_o \pm i\epsilon)\, S_\pm(E) = 1 + g^2\, V_o \cdot \left[S_\pm(E - \omega) - S_\pm(E)\right] \cdot \omega^{-1} \cdot V_o^* \,, \tag{10.150}$$

for the nucleon propagation function. (Here we replace 1_f by 1 for simplicity.)

Eq. (10.150) may be rewritten in the form

$$(E - M \pm i\epsilon)\, S_\pm(E) = 1 + g^2\, V_o \cdot S_\pm(E - \omega) \cdot \omega^{-1} \cdot V_o^* \,, \tag{10.151}$$

the self mass being identified as*

$$\Delta M = -g^2 V_o \cdot \underset{\sim}{\omega}^{-1} \cdot V_o^* \quad . \tag{10.152}$$

The renormalization constant Z_2 may be identified by passing to the limit $E \to M \mp i\epsilon$:

$$Z_2 = 1 + g^2 V_o \cdot S_\pm(M - \underset{\sim}{\omega} \mp i\epsilon) \cdot \underset{\sim}{\omega}^{-1} \cdot V_o^*$$

$$= \left[1 - g^2 V_o \cdot S_{c\pm}(M - \underset{\sim}{\omega} \mp i\epsilon) \cdot \underset{\sim}{\omega}^{-1} \cdot V_o^*\right]^{-1} . \tag{10.153}$$

Multiplication of Eq. (10.151) by Z_2^{-1} then gives

$$(E - M \pm i\epsilon)\, S_{c\pm}(E) = 1 + g^2 V_o \cdot \left[S_{c\pm}(E - \underset{\sim}{\omega}) - S_{c\pm}(M - \underset{\sim}{\omega} \mp i\epsilon)\right] \cdot \underset{\sim}{\omega}^{-1} \cdot V_o^* . \tag{10.154}$$

The simplest case in which the vertices commute is that of the <u>neutral scalar meson field</u> for which the vertex operator has the form

$$V_o = \sum_{\underset{\sim}{p}, \underset{\sim}{r}} (2\omega L^3)^{-\frac{1}{2}} v_{\underset{\sim}{p}}\, e^{i\underset{\sim}{p} \cdot \underset{\sim}{r}} f_{\underset{\sim}{r}} f_{\underset{\sim}{r}} b_{\underset{\sim}{p}} . \tag{10.155}$$

Using this form it is easy to show that the solution of Eq. (10.154) is given formally by

$$S_{c\pm}(E) = \sum_{n=0}^{\infty} \sum_{\underset{\sim}{p}_1 \cdots \underset{\sim}{p}_n} \frac{1}{n!} \left(\frac{g^2}{2L^3}\right)^n \frac{|v_{\underset{\sim}{p}_1}|^2 \cdots |v_{\underset{\sim}{p}_n}|^2}{\omega_1^3 \cdots \omega_n^3} \frac{1}{E - \omega_1 - \cdots - \omega_n - M \pm i\epsilon} \tag{10.156}$$

The integrations involved in each term of this series converge even in the limit of infinite cut-off $(v_{\underset{\sim}{p}} = 1)$. The renormalization constant Z_2, however, goes to zero as the cut-off becomes infinite, showing that the

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* Eq. (10.152) may be compared with Eq. (10.119), from which it differs by the characteristic self-energy factor $\frac{1}{2}$. In Eq. (10.152) the dot products involve summations over f-space as well as b-space.

unrenormalized quantities themselves diverge. Substitution of (10.156) into (10.153) gives, in fact,

$$Z_2 = \exp(-g^2\, V_o \cdot \underset{\sim}{\omega}^{-2} \cdot V_o^*)$$

$$\exp\left\{-(g/2\pi)^2\left[\log(2\Omega/\mu) - 1\right]\right\}$$

$$= (\mu e/2\Omega)^{(g/2\pi)^2} \tag{10.157}$$

where Ω is the high-energy cut-off.

It is of interest to take the Fourier transform of (10.156), which is easily seen to be

$$S_{c\pm}(t) = \mp i\, \theta_\pm(t)\, e^{-iMt} \exp(g^2\, V_o \cdot \underset{\sim}{\omega}^{-2} \cdot e^{-i\underset{\sim}{\omega} t} \cdot V_o^*) . \tag{10.158}$$

With infinite cut-off the exponent on the right has the form

$$(g/2\pi)^2 \int_\mu^\infty \omega^{-2}(\omega^2 - \mu^2)^{\frac{1}{2}}\, e^{-i\omega t}\, d\omega$$

$$\longrightarrow (g/2\pi)^2\left[\log(2/|\mu t|) - \gamma - 1 \mp \tfrac{1}{2}\pi i\right] \quad \text{as } t \to 0 , \tag{10.159}$$

where $\gamma = .577\ldots$, and therefore

$$S_{c\pm}(t) \longrightarrow \mp i\, \theta_\pm(t)\, e^{\mp i(g^2/8\pi)\left[2e^{-(\gamma+1)}/|\mu t|\right](g/2\pi)^2}\, e^{-iMt} \tag{10.160}$$

as $t \to 0$. From the behavior of $S_{c\pm}(t)$ near the origin one sees that the series (10.156), which is its formal Fourier transform, can converge only if $g < 2\pi$. For larger values of the coupling constant the nucleon propagation function $S_{c\pm}(E)$ must be defined by analytic continuation.

Although these results are of some interest, the neutral scalar meson problem is otherwise quite trivial. For example, the mesons are not scattered

by the nucleons. This follows from the circumstance that the operators $\bar{\mathcal{U}}_c(0, -\infty)$ and $\bar{\mathcal{U}}_c(0, \infty)$ are identical, being given, in fact, by

$$\bar{\mathcal{U}}_c(0, \mp\infty) = \exp\left[g\,\bar{\Psi}^* \cdot (V_o \cdot \underset{\sim}{\omega}^{-1} \cdot a - a^* \cdot \underset{\sim}{\omega}^{-1} \cdot V_o^*) \cdot \bar{\Psi} \right] . \tag{10.161}$$

To show that this operator diagonalizes the total Hamiltonian operator, first take its commutator with H_o. Since the vertices commute the nucleon field variables play no role in the commutation procedure, and one finds

$$\begin{aligned}
\left[H_o, \bar{\mathcal{U}}_c(0, \mp\infty) \right] &= \left[a^* \cdot \underset{\sim}{\omega} \cdot a, \bar{\mathcal{U}}_c(0, \mp\infty) \right] \\
&= - H_1 \bar{\mathcal{U}}_c(0, \mp\infty) - g \left[\bar{\mathcal{U}}_c(0, \mp\infty), \bar{\Psi}^* \cdot V_o \cdot a \cdot \bar{\Psi} \right] \\
&= - H_1 \bar{\mathcal{U}}_c(0, \mp\infty) - g^2 \bar{\mathcal{U}}_c(0, \mp\infty)(\bar{\Psi}^* \cdot V_o \cdot \bar{\Psi}) \cdot \underset{\sim}{\omega}^{-1} \cdot (\bar{\Psi}^* \cdot V_o^* \cdot \bar{\Psi})
\end{aligned}$$

and hence (cf. Eq. (6.29))

$$\bar{\mathcal{U}}_c(\mp\infty, 0)\, H\, \bar{\mathcal{U}}_c(0, \mp\infty) = H_o - g^2 (\bar{\Psi}^* \cdot V_o \cdot \bar{\Psi}) \cdot \underset{\sim}{\omega}^{-1} \cdot (\bar{\Psi}^* \cdot V_o^* \cdot \bar{\Psi}) . \tag{10.162}$$

The second term on the right gives the interaction energy between nucleons, plus the nucleon self-energy which has already been identified by Eq. (10.152). The renormalization constant Z_2 may be obtained directly from expression (10.161). We have

$$\begin{aligned}
Z_2^{\frac{1}{2}} &= \langle N_o | N \rangle = \langle N_o | \bar{\mathcal{U}}_c(0, \mp\infty) | N_o \rangle \\
&= \left\langle 0 \left| \exp\left[g(V_o \cdot \underset{\sim}{\omega}^{-1} \cdot a - a^* \cdot \underset{\sim}{\omega}^{-1} \cdot V_o^*) \right] \right| 0 \right\rangle \\
&= \sum_{n=0}^{\infty} (-1)^n \frac{(2n)!}{2^n\, n!} \frac{g^{2n}}{(2n)!} (V_o \cdot \underset{\sim}{\omega}^{-2} \cdot V_o^*)^n
\end{aligned} \tag{10.163}$$

which leads immediately to (10.156). Here the factor $(2n)!/(2^n\, n!)$ indicates

the number of different ways in which n creations can be paired off with n annihilations.*

A still more trivial example, which is nevertheless not without interest, is provided by the case in which the coupling term in the Lagrangian density for the system involves the time derivative of the meson field:

$$\mathcal{L} = i\,\underset{\sim}{\psi}^*(\dot{\underset{\sim}{\psi}} + i\,M_o\underset{\sim}{\psi}) - \tfrac{1}{2}\left[(\nabla\underset{\sim}{\phi})^2 - \dot{\underset{\sim}{\phi}}^2 + \mu^2\underset{\sim}{\phi}^2\right] + L^{-3}\,E_{vac}$$
$$- (g/\mu)\int \dot{\underset{\sim}{\phi}}'\,\rho(\underset{\sim}{r}' - \underset{\sim}{r})\,\underset{\sim}{\psi}^*\underset{\sim}{\psi}\,d^3\underset{\sim}{r}' \quad . \tag{10.164}$$

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* The same type of procedure can be used to compute all the other matrix elements of $\overline{\mathcal{U}}_c(0,\mp\infty)$. For example

$$\left\langle m \left| \overline{\mathcal{U}}_c(0,\mp\infty) \right| 0 \right\rangle = Z_2^{\frac{1}{2}}(-\,g\,\underset{\sim}{\omega}^{-1}\cdot V_o^*)^m_{sym} \;,$$

$$\left\langle m \left| \overline{\mathcal{U}}_c(0,\mp\infty) \right| 1 \right\rangle = Z_2^{\frac{1}{2}}\left[\underset{\sim}{1}_b(-\,g\,\underset{\sim}{\omega}^{-1}\cdot V_o^*)^{m-1}\right]_{sym}$$
$$+ Z_2^{\frac{1}{2}}(-\,g\,\underset{\sim}{\omega}^{-1}\cdot V_o^*)^m_{sym}(g\,V_o\cdot\underset{\sim}{\omega}^{-1}) \;, \text{ etc.,}$$

where the notation "sym" indicates that a sum over all permutations of the m final mesons is to be taken. Here only one nucleon is assumed to be present. It is easy to see that <u>all</u> matrix elements involve the factor $Z_2^{\frac{1}{2}}$ or powers of it. When the cut-off becomes infinite so that Z_2 vanishes, this would seem to imply that <u>all</u> the perturbed states are <u>orthogonal</u> to <u>all</u> the unperturbed states (with the exception, of course, of the vacuum state). This circumstance has sometimes led to the assertion that H_o and H operate in different vector spaces [113, 114]. Such an interpretation, however, is incorrect. The operators $\overline{\mathcal{U}}_c(0,\mp\infty)$ are always unitary, and the phenomenon simply shows that when the cut-off is infinite, the switching on of the perturbation spreads a given state infinitely thinly over an infinite number of other states.

The Hamiltonian operator for this system has the form

$$H = M_o \Psi^* \cdot \Psi + a^* \cdot \underset{\sim}{\omega} \cdot a - i(g/\mu) \Psi^* \cdot (V_o \cdot \underset{\sim}{\omega} \cdot a - a^* \cdot \underset{\sim}{\omega} \cdot V_o^*) \cdot \Psi$$

$$+ (g/\mu)^2 (\Psi^* \cdot V_o \cdot \Psi) \cdot \underset{\sim}{\omega} \cdot (\Psi^* \cdot V_o^* \cdot \Psi) \qquad (10.165)$$

and is diagonalized by the operator

$$\bar{\mathcal{U}}_c(0, \mp\infty) = \exp\left[- i(g/\mu) \Psi^* \cdot (V_o \cdot a + a^* \cdot V_o^*) \cdot \Psi \right], \qquad (10.166)$$

which gives

$$\bar{\mathcal{U}}_c(\mp\infty, 0)\, H\, \bar{\mathcal{U}}_c(0, \mp\infty) = H_o . \qquad (10.167)$$

In this case there is not even any interaction between the nucleons themselves.

This system, in spite of its triviality, may be analyzed in a nontrivial fashion by the methods previously developed. It is only necessary to replace the quantities g, V_o, V_o^*, everywhere they previously occurred, respectively by g/μ, $-i\, V_o \cdot \underset{\sim}{\omega}$, $i\underset{\sim}{\omega} \cdot V_o^*$. In addition, since the self mass now vanishes, it is necessary to add a term $(g/\mu)^2\, V_o \cdot \underset{\sim}{\omega} \cdot V_o^*$ to the right hand side of Eq. (10.149). The renormalized propagation function is given again by Eq. (10.156) with the functions $v_{\underset{\sim}{p}}$ replaced by $-i\omega v_{\underset{\sim}{p}}$.

The interest possessed by this example appears when the cut-off is allowed to become infinite. The individual terms of the renormalized series (10.156) <u>no longer converge</u> on account of the extra factors ω^2 in the numerators. However, its Fourier transform is still well defined, being given by

$$S_{c\pm}(t) = \mp i\, \theta_\pm(t)\, e^{-iMt} \exp\left[(g/\mu)^2\, V_o \cdot e^{-i\underset{\sim}{\omega} t} \cdot V_o^* \right] . \qquad (10.168)$$

The exponent on the right now has the form

$$(g/2\pi\mu)^2 \int_\mu^\infty (\omega^2 - \mu^2)^{\frac{1}{2}} e^{-i\omega t}\, d\omega$$

$$\longrightarrow (g/2\pi)^2 \left[-(\mu t)^{-2} + \tfrac{1}{2} \log (|\mu t|/2) \pm \tfrac{1}{4}\pi i \right] \quad \text{as} \quad t \to 0 \ , \tag{10.169}$$

and therefore

$$S_{c\pm}(t) \longrightarrow \mp i\, \theta_\pm(t)\, e^{\pm i(g^2/16\pi)\left[\frac{1}{2}|\mu t| \; e^{-2(\mu t)^{-2}} \right] \frac{1}{2}(g/2\pi)^2} e^{iMt} \tag{10.170}$$

as $t \to 0$. The function $S_{c\pm}(t)$ evidently has a perfectly respectable Fourier transform. However, this transform <u>cannot be expended in powers of</u> g^2, since if g^2 is replaced by $-g^2$ then $S_{c\pm}(t)$ does not vanish at the origin but has an essential singularity there instead. This is the reason for the present lack of convergence of the terms of the series (10.156).

The present example perhaps throws some light on the situation occurring in the so-called nonrenormalizable theories, [111, 112] which are characterized, as here, by "derivative coupling" and by the lack of convergence of even the individual terms in the expansions of renormalized quantities.*

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* The dependence of the renormalization constant on the cut-off is given in this example by

$$Z_2 = \exp\left[-(g/\mu)^2 V_o \cdot V_o^* \right] \longrightarrow \left[2(\Omega/\mu) e^{-(\Omega/\mu)^2} \right]^{\frac{1}{2}(g/2\pi)^2} .$$

11. DECAYING SYSTEMS AND RESONANCE SCATTERING

Unstable states.

Suppose the system H is known to be in the eigenstate $|\alpha_o'\rangle$ of H_o at the time $t = 0$. Then the probability that it will be found in the same state at a later time t is $\left|\langle\alpha_o'|\bar{U}(t, 0)|\alpha_o'\rangle\right|^2$. The state $|\alpha_o'\rangle$ is said to be unstable for the system H if

$$\lim_{t\to\infty} \left|\langle\alpha_o'|\bar{U}(t, 0)|\alpha_o'\rangle\right|^2 = 0 , \tag{11.1}$$

the limit being taken in a straightforward manner independent of any special conventions. Otherwise the state is said to be stable. A system which is initially in an unstable state is said to undergo a subsequent decay.

An unstable initial state is often referred to as an excited state, the implication being that some kind of previous excitation process has taken place which puts the system into the state in question. In practice it is usually an experimental impossibility to put the system H into a pure unstable eigenstate of the most convenient reference system H_o at a given instant of time. However, the subsequent behavior of the hypothetical initially pure state is generally sufficiently descriptive of the actual state of affairs, at least after an initial "settling down" time has elapsed, for the adjective "excited" to be applied to it directly.

If the average value of the Green's function $G_\pm(E)$ in the state $|\alpha_o'\rangle$ is known, then the time dependence of the amplitude $\langle\alpha_o'|\bar{U}(t, 0)|\alpha_o'\rangle$ can be determined from the relation

$$\langle \alpha_o' | \bar{U}(t, 0) | \alpha_o' \rangle = e^{iE't} \langle \alpha_o' | U(t, 0) | \alpha_o' \rangle$$

$$= \begin{cases} -(2\pi i)^{-1} \int_{-\infty}^{\infty} \langle \alpha_o' | G_+(E) | \alpha_o' \rangle e^{i(E' - E)t} dE, & t > 0, \\ (2\pi i)^{-1} \int_{-\infty}^{\infty} \langle \alpha_o' | G_-(E) | \alpha_o' \rangle e^{i(E' - E)t} dE, & t < 0, \end{cases} \tag{11.2}$$

(Here E' refers to the spectrum of H_o.) An examination of the diagonal matrix elements of the Green's function therefore allows one to determine the stability for H of the various eigenstates of H_o and the decay rates of those states which are unstable.

The damping operator.

The special significance possessed by the diagonal matrix elements of the Green's function in decay problems is analogous to that possessed by the particle propagation functions of field theories. One may exploit this analogy by introducing a generalization of the self-energy function (or mass operator) which has been called by Heitler the damping operator. [68, 69, 86]

First, denote by F_d and F_{od} respectively the diagonal and off-diagonal parts of a given operator F; i.e.

$$F_d = \sum{}' |\alpha_o'\rangle \langle \alpha_o' | F | \alpha_o' \rangle \langle \alpha_o' | , \tag{11.3}$$

$$F_{od} = F - F_d . \tag{11.4}$$

Then, using this notation and the fact that $G_{o\pm}(E) = \left[G_{o\pm}(E)\right]_d$, separate the right hand side of Eq. (2.15) into diagonal and off-diagonal parts as follows:

$$G_{\pm}(E) = G_{o\pm}(E)\left\{1 + H_1\left[G_{\pm}(E)\right]_d + H_1\left[G_{\pm}(E)\right]_{od}\right\}$$

$$= G_{o\pm}(E)\left\{1 + D_{\pm}(E)\left[G_{\pm}(E)\right]_d\right\}, \tag{11.5}$$

where

$$D_{\pm}(E) = H_1\left\{1 + G_{o\pm}(E)\left[D_{\pm}(E)\right]_{od}\right\}. \tag{11.6}$$

$D_{\pm}(E)$ is the damping operator. Comparison of Eqs. (11.6) and (7.4a) shows that it is closely related to the operator $R_{\pm}(E)$. Iteration of Eq. (11.6) gives

$$\left\langle \alpha_o'' \middle| D_{\pm}(E) \middle| \alpha_o' \right\rangle = \left\langle \alpha_o'' \middle| H_1\left[1 - \left(1 - \left|\alpha_o'\right\rangle\left\langle\alpha_o'\right|\right)G_{o\pm}(E)H_1\right]^{-1} \middle| \alpha_o' \right\rangle \tag{11.7}$$

The self-energy function is the diagonal part of the damping operator:

$$\Sigma_{\pm}(E) = \left[D_{\pm}(E)\right]_d = \Sigma_{\mp}(E)^* . \tag{11.8}$$

In terms of it the diagonal part of the Green's function may be written

$$\left[G_{\pm}(E)\right]_d = \left[E - H_o - \Sigma_{\pm}(E) \pm i\epsilon\right]^{-1} . \tag{11.9}$$

By reasoning identical with that of the preceding section in connection with the nucleon propagation function, one easily sees that the spectrum of the operator H is given by the poles of $\left[G_{\pm}(E)\right]_d$ on the real axis in the limit $\epsilon \to 0$. That is, the eigenvalues E' of H are the real solutions of the equations

$$\lim_{\epsilon \to 0}\left[E - H_o' - \Sigma_{\pm}'(E) \pm i\epsilon\right] = 0 \tag{11.10}$$

where

$$\Sigma_{\pm}'(E) = \left\langle \alpha_o' \middle| D_{\pm}(E) \middle| \alpha_o' \right\rangle . \tag{11.11}$$

When decay problems are involved, some of the equations (11.10) have no real solutions. It will be seen presently that the corresponding eigenstates of H_o are the unstable states and have, therefore, no counterparts in the system H. In Section 7 we briefly considered the situation presented by such states in connection with the S-matrix and denoted them there by $|\gamma_o'\rangle$. The remaining (stable) states were denoted by $|\beta_o'\rangle$. We now proceed to investigate these two classes of states in greater detail.

Real solutions.

We consider first the stable states $|\beta_o'\rangle$ for which the equations (11.10) have real solutions E'. Prompted by our experience with propagation functions in field theories, we expand $\Sigma_\pm'(E)$ about the point $E' \mp i\epsilon$:

$$\Sigma_\pm'(E) = \Delta E' - \zeta'(E - E' \pm i\epsilon) \quad \text{Rem } \Sigma_\pm'(E) , \tag{11.12}$$

$$\Delta E' = \left[\Sigma_\pm'(E)\right]_{E=E' \mp i\epsilon} , \tag{11.13}$$

$$\zeta' = -\left[\partial \Sigma_\pm'(E)/\partial E\right]_{E=E' \mp i\epsilon} . \tag{11.14}$$

The constants $\Delta E'$ are, of course, the level shifts, satisfying

$$\begin{aligned} E' &= H_o' + \Delta E' \\ &= H_o' + \lim_{\epsilon \to 0} \langle \beta_o'| H_1 \left[1 - \left(1 - |\beta_o'\rangle\langle\beta_o'|\right) G_{o\pm}(E') H_1\right]^{-1} |\beta_o'\rangle , \end{aligned} \tag{11.15}$$

which may be compared with Eq. (9.58) of bound state perturbation theory. The ζ' are related to the normalization constants Z' by the now familiar equation

$$Z' = (1 + \zeta')^{-1} . \tag{11.16}$$

It is instructive, in the present section, to rederive Eq. (11.16) by methods employing the damping operator directly. Adding the off-diagonal part of Eq. (11.5) to the identity $\left[G_{\pm}(E)\right]_d = \left[G_{\pm}(E)\right]_d$, one gets

$$G_{\pm}(E) = \left\{1 + G_{0\pm}(E)\left[D_{\pm}(E)\right]_{od}\right\}\left[G_{\pm}(E)\right]_d \qquad (11.17)$$

Use of this result together with Eqs. (11.9) and (11.12) in Eq. (6.8) gives for the eigenvectors $|\beta_{\pm}'\rangle$ of H the expression

$$\begin{aligned} Z'^{\frac{1}{2}}|\beta_{\pm}'\rangle &= \pm i\epsilon G_{\pm}(E')|\beta_0'\rangle \\ &= (1+\zeta')^{-1}\left\{1 + G_{0\pm}(E')\left[D_{\pm}(E')\right]_{od}\right\}|\beta_0'\rangle \end{aligned} \qquad (11.18)$$

Multiplication on the left by $\langle\beta_0'|$ leads to Eq. (11.16).

Complex solutions.

If one replaces $|\beta_0'\rangle$ by $|\gamma_0'\rangle$ in the first line of Eq. (11.18) then one obtains an explicit statement of the fact that the unstable states undergo a mathematical as well as physical decay when the perturbation H_1 is switched on, or in other words that $Z' = 0$ for the $|\gamma_0'\rangle$. For there is no real value of E for which $\pm i\epsilon G_{\pm}(E)|\gamma_0'\rangle$ does not vanish in the limit $\epsilon \to 0$, since such a value would be a real solution of Eq. (11.10) for the state $|\gamma_0'\rangle$.

One may, in fact, infer that there is not even a complex value of E for which $\pm i\epsilon G_{\pm}(E)|\gamma_0'\rangle$ remains finite in the limit. For if there were, then this value would have to be an eigenvalue of H, which is contrary to the hypothesis that H is Hermitian. This means that Eq. (11.10) for an unstable state $|\gamma_0'\rangle$ has no solution at all, if the quantities appearing in it are evaluated in a straightforward manner. This fact will subsequently be seen to be the greatest single complicating factor in the theory of decaying

systems, causing us in many cases to be able to speak only in approximate terms and to write only approximate equations valid under restrictive conditions.

The fact that Eq. (11.10) has no solutions for unstable states may actually be shown in a direct manner. We note first that the $\pm$ signs become superfluous when E takes on complex values. (Their original purpose was simply to distinguish between values of E just above and just below the real axis.) Therefore we write simply

$$E' - H_o' - \Sigma'(E') = 0 , \tag{11.19}$$

assuming the existence of an E' satisfying this equation, and then show that this leads to a contradiction.

Using Eqs. (11.5) and (11.11) (without the $\pm$ signs) we have

$$\begin{aligned}
2 \operatorname{Im} E' &= 2 \operatorname{Im} \Sigma'(E') \\
&= -i \left\langle \gamma_o' \middle| \left[D(E') - D(E')^* \right] \middle| \gamma_o' \right\rangle \\
&= -i \left\langle \gamma_o' \middle| \left\{ H_1 G_o(E') \left[D(E') \right]_{od} - \left[D(E') \right]_{od}^* G_o(E'^*) H_1 \right\} \middle| \gamma_o' \right\rangle \\
&= -i \left\langle \gamma_o' \middle| \left[D(E') \right]_{od}^* \left[G_o(E') - G_o(E'^*) \right] \left[D(E') \right]_{od} \middle| \gamma_o' \right\rangle \\
&= -2 \operatorname{Im} E' \sum_{\alpha_o'' \neq \gamma_o'}{}'' \frac{\left| \left\langle \alpha_o'' \middle| D(E') \middle| \gamma_o' \right\rangle \right|^2}{(\operatorname{Re} E' - H_o'')^2 + (\operatorname{Im} E')^2} .
\end{aligned} \tag{11.20}$$

In the passage from the third to the fourth line of this equation H_1 is replaced by

$$D(E') - H_1 G_o(E') \left[D(E') \right]_{od} = D(E')^* - \left[D(E') \right]_{od}^* G_o(E'^*) H_1 .$$

If we now divide Eq. (11.20) by $\operatorname{Im} E'$, which is permissible since $\left| \gamma_o' \right\rangle$ is an unstable state, we obtain a positive number on the left and a negative quantity on the right, which is the contradiction sought for.

The situation is clarified by considering the classic example of the nonrelativistic radiative decay of an excited atom. The unstable initial state may be denoted by $|J_o'\rangle$, describing a bound electronic configuration in the absence of photons. The perturbation H_1 is the usual electromagnetic coupling which can emit or absorb photons only singly.* Its only nonvanishing matrix elements connecting the state $|J_o'\rangle$ are $\langle \alpha_o'', \zeta_o'' | H_1 | J_o' \rangle$ and their complex conjugates, where the label ζ_o'' describes a single photon and the label α_o'' refers to the electronic state, either bound, mixed or free. Since electromagnetic coupling is weak the diagonal elements of Eq. (11.7) are given to good approximation by

$$\Sigma_{\pm}'(E) \approx \langle J_o' | H_1 \left(1 - |J_o'\rangle \langle J_o'|\right) G_{o\pm}(E)\, H_1 | J_o' \rangle$$

$$= \sum{}'' \frac{|\langle \alpha_o'', \zeta_o'' | H_1 | J_o' \rangle|^2}{E - H_o'' \pm i\epsilon} \tag{11.21}$$

The behavior of this function off the real axis is easily inferred in terms of a physical analog. Dropping the $\pm$ signs one may write

$$\begin{aligned} \mathrm{Re}\ \Sigma'(E) &= \mathcal{E}_x(E) , \\ \mathrm{Im}\ \Sigma'(E) &= -\mathcal{E}_y(E) , \end{aligned} \tag{11.22}$$

where $\mathcal{E}_x$ and $\mathcal{E}_y$ are the components of a 2-dimensional electrostatic field produced by a charge density of amount

$$\rho(E) = \tfrac{1}{2} \sum{}'' \delta(E - H_o'') \left| \langle \alpha_o'', \zeta_o'' | H_1 | J_o' \rangle \right|^2 \tag{11.23}$$

---

* We omit the term quadratic in the electromagnetic field, which occurs in the nonrelativistic theory, since it is of higher order in the electric charge.

distributed along the real axis. Since $\rho(E)$ is non-negative one has

$$\begin{aligned} &\mathrm{Im}\ \Sigma'(E) < 0 \qquad \text{for} \qquad \mathrm{Im}\ E > 0\,, \\ &\mathrm{Im}\ \Sigma'(E) > 0 \qquad \text{for} \qquad \mathrm{Im}\ E < 0\,, \end{aligned} \tag{11.24}$$

which shows again that Eq. (11.10) has no solution.

Eq. (11.10) can, however, have a solution if a process of analytic continuation is carried out on the function $\Sigma'(E)$. This function evidently has a branch point at E_{min}, where E_{min} is the lowest lying of the levels H_o'' for which the numerator in the sum (11.21) is nonvanishing. Eq. (11.21) defines this function only over one of its Riemann sheets, and although Eq. (11.10) has no solution on this sheet it generally has solutions on the next adjoining sheets. Use of Eq. (11.21) to define the function $\Sigma'(E)$ implies a cut along the real axis starting at E_{min}. One can get onto the adjacent Riemann sheets by displacing this cut either upwards or downwards. The $\pm$ signs will now be reinstated so as to refer to the appropriate adjacent sheet. The function $\Sigma_+(E)$ is obtained by displacing the cut downward, or alternatively by crossing the cut from above. Similarly, the function $\Sigma_-(E)$ is obtained by displacing the cut upward, etc.

The real part of Eq. (11.21) is usually divergent. In terms of the electrostatic analog this means that the total charge $\int \rho(E)dE$ is not only infinite but also distributed at large distances in such a way that the component $\mathcal{E}_x$ of the electric field is negatively infinite. We shall avoid this difficulty by the usual procedure of introducing a high energy cut-off, which we shall call E_{max}. E_{max} is evidently also a branch point. For general systems there may be other branch points on the real axis, particularly when the exact formula (11.7) is used for computing $\Sigma'(E)$ to an arbitrarily high order. In order to avoid extra complications in this section, however,

we shall assume that E_{min} and E_{max} are the only two branch points and that the Riemann cut connects them. If formula (11.21) is used as exact this means that the charge density $\rho(E)$ is infinitely differentiable everywhere along the cut.

Fig. 15 shows how the cut is to be displaced so as to obtain the function $\Sigma_+'(E)$. The contour C_+ lying just above the real axis is deformed into a contour $-C_{min} + C_- - C_{max}$. Similarly Fig. 16 shows the displacement of the cut which defines the function $\Sigma_-'(E)$. The contour C_- lying just below the real axis is deformed into the contour $C_{min} + C_+ + C_{max}$.

Since the functions $\Sigma_\pm'(E)$ are analytic over their respective sheets one may write

$$\Sigma_\pm(E) = \Sigma_\mp(E^*)^* \quad , \tag{11.25}$$

since, by (11.8), the equation holds on the real axis. The solutions (which now exist) to the equations

$$E_\pm' - H_o' - \Sigma_\pm'(E') = 0 \tag{11.26}$$

therefore satisfy the conjugate relationship

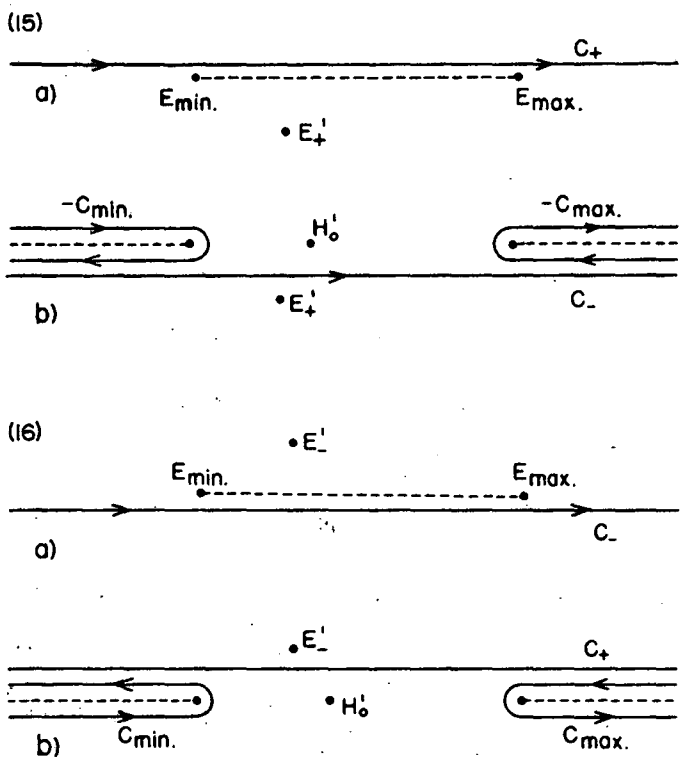
$$E_\pm' = E_\mp'^* \quad . \tag{11.27}$$

Eq. (11.26) may have several solutions in a given Riemann sheet. There will generally, however, be a principal one which lies closest to the real axis and passes to H_o' as $g \to 0$, and this is the one we shall consider, ignoring the rest.

E_+' and E_-' lie in the lower and upper half-planes respectively, and one may therefore write

$$E_\pm' = H_o' + \Delta E' \mp \tfrac{1}{2} i\Gamma' \quad , \tag{11.28}$$

where Γ' is a positive constant. $\Delta E'$ and Γ' are known respectively as the <u>shift</u> and <u>width</u> of the perturbed energy level corresponding to the state $|\gamma_o'\rangle$,



FIGS. 15 & 16 SHOWING THE DISPLACEMENTS OF CONTOUR AND CUT, WHICH DEFINE THE FUNCTIONS $\Sigma'_{\pm}(E)$

MU-10088

although there is now no strict mathematical justification for this nomenclature since $|\gamma_0'\rangle$ has no counterpart in H. However, there is ample physical justification, as will presently appear, and it will be convenient in the subsequent discussion to introduce a redefined perturbation operator $\mathcal{H}_1$ (see Eqs. (6.4, 5, 6)) such that the eigenvalues of the modified unperturbed Hamiltonian $\mathcal{H}_0$ are given by

$$E' = H_0' + \Delta E' \tag{11.29}$$

for the unstable as well as the stable states. In the S-matrix discussion of Section 7 only the stable-level redefinition was considered.

A remark should be made about the level redefinition procedure. In a relativistic local field theory involving only free particles the level shifts are both infinite and unobservable. In a decay situation, however, in which a nonrelativistic feature in the form of an external binding potential is present, there is, for states involving bound particles, a finite part of the level shift which <u>is</u> observable. It is important to remember that the level redefinition (11.29) includes not only the unobservable contribution corresponding to the free particle situation but also the observable part arising from the passage to a bound (or mixed) state.

<u>Discussion of instability.</u>

For unstable states, just as for stable states, it is convenient to expand $\Sigma_\pm'(E)$. Remembering that the perturbation operator has now been redefined so that $\Delta E' = 0$, one has

$$\Sigma_\pm'(E) = \mp \tfrac{1}{2} i \Gamma' - \zeta_\pm'(E - E_\pm') + \text{Rem } \Sigma_\pm'(E) \tag{11.30}$$

where

$$\zeta_\pm' = - \left[\partial \Sigma_\pm'(E)/\partial E \right]_{E=E_\pm'} . \tag{11.31}$$

The quantity

$$Z_{\pm}' = (1 + \zeta_{\pm}')^{-1} \tag{11.32}$$

will be seen to play a physical role analogous to that of the renormalization constants for stable states, although here again the strict mathematical justification for an interpretation along such lines is lacking.

Evidently ζ_+' and ζ_-' are complex conjugates of one another, and one may write

$$\zeta_{\pm}' = \zeta' \pm i\eta' \tag{11.33}$$

where ζ' and η' are real constants. It is useful to introduce also the quantity

$$Z' = (1 + \zeta')^{-1} \quad , \tag{11.34}$$

in terms of which one has

$$Z_{\pm}' = Z'(1 \pm i\eta_c')^{-1} \quad , \tag{11.35}$$

$$\eta_c' = Z'\eta' \quad . \tag{11.36}$$

The Z' here is not to be confused with the strictly vanishing normalization constant which expresses the fact that $|\gamma_0'\rangle$ has no counterpart in H. If the perturbation H_1 (or $\mathcal{H}_1$) is weak then generally

$$|\eta_c'| \ll 1 \quad , \tag{11.37}$$

and the $Z_{\pm}'$ are nearly equal to Z'.

Now, set $E = E'$ in Eq. (11.30) and take the imaginary part, getting

$$\mp 2 \text{ Im } \Sigma_{\pm}'(E') = Z'^{-1}\Gamma' \mp 2 \text{ Im Rem } \Sigma_{\pm}'(E') \ . \tag{11.38}$$

Since E' is real it lies on the original Riemann sheet defining the function $\Sigma'(E)$, and hence the left hand side of this equation may be evaluated in the straightforward manner of Eq. (11.20). Reinserting the $\pm$

signs into the latter equation, and using the fact that

$$G_{o\pm}(E') - G_{o\mp}(E') = \mp 2\pi i\, \delta(E' - \mathcal{H}_o) ,$$

one gets

$$\Gamma' = 2\pi Z' \sum_{\alpha_o'' \neq \gamma_o'}{}'' \delta(E' - E'') \left| \langle \alpha_o'' | D_\pm(E') | \gamma_o' \rangle \right|^2 \pm 2 \operatorname{Im} \Sigma_{c\pm}'(E') + 2\, \eta_c' \operatorname{Re} \Sigma_{c\pm}'(E') \tag{11.39}$$

where (cf. Eq. (10.75))

$$\Sigma_{c\pm}'(E) = Z_\pm' \operatorname{Rem} \Sigma_\pm'(E) . \tag{11.40}$$

If the perturbation is weak then Γ' is small and the terms in $\Sigma_{c\pm}'(E')$ (which are of order Γ'^2 and Γ'^3 respectively) may be neglected in (11.39). Comparison with Eq. (8.12) then suggests that Γ' may have an approximate interpretation as the <u>total rate of transition out of the state</u> $|\gamma_o'\rangle$. This interpretation will subsequently be more fully confirmed.

Eq. (11.39) allows one immediately to infer the characteristics which distinguish the stable states from the unstable ones and which have already been indicated in Section 3. First of all, an unstable state $|\gamma_o'\rangle$ cannot be a free state, for the matrix element

$$\langle \gamma_o' | \left[D_\pm(E') \right]_{od}^* \delta(E' - \mathcal{H}_o) \left[D_\pm(E') \right]_{od} | \gamma_o' \rangle$$

would then be inversely proportional to some positive power of the dimension L of the normalizing box and hence vanish in the limit $\epsilon \to 0$, $L \to \infty$. Secondly, if $|\gamma_o'\rangle$ is a mixed state representable, for example, as $|J_o', \zeta_o'\rangle$, then the operator $\left[D_\pm(E') \right]_{od}$ must have some nonvanishing matrix elements of the form $\langle \alpha_o'', \zeta_o' | D_\pm(E') | J_o', \zeta_o' \rangle$ which depend on L only through the labels α_o''. That is, the bound subsystem described

by the labels J_o' must play the essential decay role, for only then can the summation over the labels α_o'' in Eq. (11.39) remove the L dependence of Γ'. Finally, owing to the presence of the delta function in Eq. (11.39), the labels α_o'' which give rise to the significant contributions in the sum must refer to a set of continuum levels engulfing the energy level of the state $|\gamma_o'\rangle$. Obviously, the classical radiative decay example fits all these requirements, the engulfing continuum being provided by the emitted photons. One sees in general that, of the bound electronic levels, only the lowest lying are stable. The free electronic states, on the other hand, are stable, photon production in this case giving rise merely to inelastic scattering processes.*

The decay process.

To obtain the temporal behavior of an excited state $|\gamma_o'\rangle$ one substitutes Eq. (11.9) into Eq. (11.2) and then deforms the integration contour in the manner shown in Figs. 15 or 16. We shall consider the case $t > 0$, the case $t < 0$ being obtainable from it by the relation

$$\langle \alpha_o' | \bar{\mathcal{U}}(-t, 0) | \alpha_o' \rangle = \langle \alpha_o' | \bar{\mathcal{U}}(t, 0) | \alpha_o' \rangle^* . \qquad (11.41)$$

(Here the substitution $H_o \rightarrow \mathcal{H}_o$ has been made.) Using Eq. (11.30) and ignoring any poles in the lower half plane other than the one at E_+', one has

$$\langle \gamma_o' | \bar{\mathcal{U}}(t, 0) | \gamma_o' \rangle = -\frac{1}{2\pi i}\left(\int_{C_-} - \int_{C_{min}} - \int_{C_{max}}\right)\frac{e^{i(E'-E)t}}{E - E' - \Sigma_+'(E)}\, dE$$

$$= Z_+' e^{-\frac{1}{2}\Gamma' t} + \frac{Z_+'}{2\pi i}\left(\int_{C_{min}} + \int_{C_{max}}\right)\frac{e^{i(E'-E)t}}{E - E' - \Sigma_{c+}'(E)}\, dE . \qquad (11.42)$$

---

* The relation between Γ' and Im $\Sigma_\pm'(E')$ is obviously a generalization of the relation, in scattering theory, between the total cross section and the imaginary part of the forward scattering amplitude (Eq. (8.33)).

The first term on the right of this equation gives the familiar exponential decay law, modified however through the presence of the normalization factor Z_+'. Since the entire expression must equal unity at $t = 0$, the second term on the right must describe various transient effects. This term starts out with the value $1 - Z_+'$, and then normally drops quickly to very small values. The "settling down time" depends to a considerable extent on the details of the specific system involved, and only a very crude estimate of it can be given in general. The estimate is obtained by writing one of the contour integrals, the integral over C_{min} for instance, in the form

$$\frac{1}{2\pi i}\int_{-\infty}^{E_{min}} \frac{\left[\Sigma_{+-}'(E) - \Sigma_{++}'(E)\right] e^{i(E' - E)t}}{\left[E - E' - \Sigma_{+-}'(E)\right]\left[E - E' - \Sigma_{++}'(E)\right]}\, dE \,, \tag{11.43}$$

where Σ_{+-}' and Σ_{++}' are the values of the function Σ_+' respectively below and above the cut from E_{min} to $-\infty$, and examining the breadth of the range of values E over which the integrand has significant values. If $\Sigma_{++}'(E)$ is approximated by Eq. (11.21), which allows it to be interpreted in terms of an electrostatic analog, it evidently becomes negligible in value when $E_{min} - E \gg E_{max} - E_{min}$. The same usually holds, by analytic continuation, for $\Sigma_{+-}'(E)$, and therefore $(E_{max} - E_{min})^{-1}$ may be regarded as a rough estimate of the settling down time.

For large values of t it is often convenient to make the transformation of variables $E \rightarrow x$, where $x^2 = E_{min} - E$, which changes the bent contour C_{min} into a straight line. It is then sometimes possible to make an approximate evaluation of expression (11.43) in terms of complex error functions. The chief characteristic of such functions is that their asymptotic behavior follows not an exponential law but rather an inverse

power law in t. This means that although the second term on the right of Eq. (11.42) may drop to a value smaller than that of the first term it eventually predominates again. This phenomenon has been termed a "straggling effect." [91]

In trivial cases the straggling effect may dominate the entire decay process. For example, if H_o describes a simple system having bound states as a result of an attractive potential, and if the perturbation H_1 consists of a mere switching off of this potential, then the disinherited bound states will decay by the ordinary wave-packet diffusion law, which is never exponential.

This may be illustrated by the one-dimensional delta-function example considered in Sections 8 and 9. Here the roles of the perturbed and unperturbed systems are inverted:

$$H_o = \tfrac{1}{2} p^2 - g\,\delta(\underset{\sim}{r}) , \qquad H_1 = g\,\delta(\underset{\sim}{r}) . \tag{11.44}$$

Expressions (8.85) and (8.87) are now the "unperturbed" wave functions, and one easily finds

$$\begin{aligned}
\left\langle \underset{\sim}{p}_\pm'' \middle| H_1 \middle| \underset{\sim}{p}_\pm' \right\rangle &= g\,L^{-1}\,p''(g \mp ip'')^{-1}\,p'(g \pm i\,p')^{-1} , \\
\left\langle \underset{\sim}{p}_\pm'' \middle| H_1 \middle| J' \right\rangle &= \mp i\,g^{3/2}\,L^{-\frac{1}{2}}\,p''(g \mp i\,p'')^{-1} , \\
\left\langle J' \middle| H_1 \middle| J' \right\rangle &= g^2 .
\end{aligned} \tag{11.45}$$

Substitution of these matrix elements into Eq. (11.7) gives

$$\begin{aligned}
\Sigma'(E) &= \left\langle J' \middle| H_1 \middle| J' \right\rangle + \sum{}'' \frac{\left\langle J' \middle| H_1 \middle| \underset{\sim}{p}_\pm'' \right\rangle \left\langle \underset{\sim}{p}_\pm'' \middle| H_1 \middle| J' \right\rangle}{E - \frac{1}{2} p''^2} + \cdots \\
&= g^2 \left[1 + \frac{2\,g}{\pi} \int_0^\infty \frac{p^2}{(p^2 + g^2)(p^2 - 2\,E)}\,dp \right]^{-1}
\end{aligned}$$

$$= g^2 \frac{(2E)^{\frac{1}{2}} \pm ig}{(2E)^{\frac{1}{2}} \pm 2ig} , \qquad \begin{array}{l} + \text{ sign for } \operatorname{Im} E > 0 , \\ - \text{ sign for } \operatorname{Im} E < 0 . \end{array} \tag{11.46}$$

Here there is only one branch point at $E = E_{min} = 0$. If the cut starting from E_{min} is deformed as in Figs. 15 or 16, then the choice of sign in (11.46) corresponds to the choice of function $\Sigma_{\pm}'(E)$.

Remembering that $H_0' = -\frac{1}{2} g^2$, one finds that Eq. (11.26) has two roots, namely

$$E_{\pm}' = 0 , \; -\tfrac{1}{2} g^2 . \tag{11.47}$$

The level width is evidently zero, which shows already that the case of simple "switch-off" is not an ordinary type of decay.* It <u>is</u> however a true decay as may be seen by carrying out the integration of Eq. (11.2). Introducing the variable $p^2 = 2E$, one may write, for $t > 0$,

$$\left\langle J' \middle| \bar{U}(t, 0) \middle| J' \right\rangle = -\frac{1}{2\pi i}\left(\int_{i\infty}^{0} + \int_{0}^{\infty}\right) \frac{p\, e^{-\frac{1}{2} i(p^2 + g^2)t}}{\frac{1}{2} p^2 + \frac{1}{2} g^2 - g^2(p + ig)(p + 2ig)^{-1}} dp \tag{11.48}$$

$$= -\frac{1}{\pi i}\int_{-\infty}^{\infty}\left[\frac{1}{p + ig} + \frac{ig}{(p + ig)^2}\right] e^{-\frac{1}{2}i(p^2 + g^2)t} dp$$

$$= (g/\pi)\int_{-\infty}^{\infty} dp \int_{0}^{\infty} dt'(1 + g^2 t') e^{ig(p + ig)t' - \frac{1}{2}i(p^2 + g^2)t}$$

$$= g(2/\pi t)^{\frac{1}{2}} e^{-\frac{1}{4}\pi i}\left(\int_{it}^{0} + \int_{0}^{\infty}\right)(1 - ig^2 t + g^2 t'') e^{\frac{1}{2}i(g^2/t)t''^2} dt''$$

$$= (1 - ig^2 t)\left[1 - ige^{-\frac{1}{4}\pi i}(2/\pi t)^{\frac{1}{2}}\int_{0}^{t} e^{-\frac{1}{2}i(g^2/t)x^2} dx\right] + ige^{-\frac{1}{4}\pi i}(2t/\pi)^{\frac{1}{2}} e^{-\frac{1}{2}ig^2 t}$$

---

* The vanishing of $\operatorname{Im} E_{\pm}'$ is doubtless related to the fact that the bound states of H_0 are not entirely without counterparts in H; that they pass over, in a sense, into the bottom of the set of continuum states.

Deformations of the integration contour are involved in the passage from the first to the second line and from the third to the fourth line of this equation. The variables $t'' = t' + it$ and $x = -it''$ have also been introduced. One easily gets for the asymptotic behavior the expressions

$$\left| \left\langle J' \middle| \bar{U}(t, 0) \middle| J' \right\rangle \right|^2 \longrightarrow \begin{cases} 1 - (4/3)\pi^{-\frac{1}{2}} g^3 t^{3/2} + g^4 t^2 & t \to 0 \\ 8\pi/g^2 t \,, & t \to \infty \end{cases} . \tag{11.49}$$

As far as simple systems are concerned a case of greater interest is that in which the decay is due to barrier penetration. For simplicity consider a nonrelativistic particle of unit mass which is initially trapped in a potential V which has the form indicated schematically in Fig. 17a. Here the wave packet diffusion takes place by leakage through the barrier which forms V. If this barrier is sufficiently thick the onset of the inevitable straggling behavior will be deferred to a time in the distant future so that, to all intents and purposes, the decay <u>will</u> now be exponential. The unperturbed system for which this initial state is stable may be obtained simply by placing an infinitely thick barrier B (see Fig. 17b) around the particle. This barrier must, however, affect only the bound state and not the free states. Therefore the choice of unperturbed Hamiltonian must be somewhat artificial, for example

$$H_o = H_{oo} - h\,\overline{\theta_+}(H_{oo} - h) \tag{11.50}$$

where h is the height of the barrier B and

$$H_{oo} = \tfrac{1}{2} p^2 + V + B \,. \tag{11.51}$$

Since the Hamiltonian operator of the actual system is $H = \frac{1}{2} p^2 + V$, the perturbation operator is

$$H_1 = -B + h\,\theta_+(H_{oo} - h) \,. \tag{11.52}$$

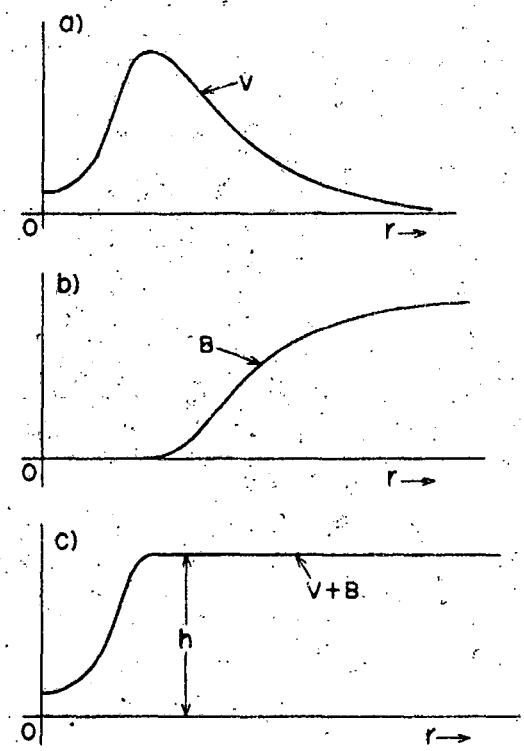


FIG. 17:

a) A POTENTIAL BARRIER V THROUGH WHICH LEAKAGE CAN OCCUR

b) AN INFINITELY THICK BARRIER B THROUGH WHICH NO LEAKAGE CAN OCCUR

c) THE SUM OF V AND B

MU-10089

Denoting the bound state by $|J_o'\rangle$ and the free states by $|\zeta_o''\rangle$, one may therefore write for the self-energy function the expansion

$$\Sigma_\pm'(E) = -\langle J_o'|B|J_o'\rangle + \sum{}'' \frac{|\langle \zeta_o''|B|J_o'\rangle|^2}{E - E'' \pm i\epsilon}$$

$$+ \sum{}''' \frac{\langle J_o'|B|\zeta_o'''\rangle \langle \zeta_o'''|(h-B)|\zeta_o''\rangle \langle \zeta_o''|B|J_o'\rangle}{(E - E''' \pm i\epsilon)(E - E'' \pm i\epsilon)} + \cdots \tag{11.53}$$

the E'' being the eigenvalues of H_o. If the barrier which forms V is quite thick, so that the wave function corresponding to $|J_o'\rangle$ penetrates very little into B, it is evident that $\Sigma_\pm'(E)$ is small.*

By proper choice of B in the above example the initial transient effects may be largely eliminated, which means that the normalization constants $Z_\pm'$ may be brought close to unity in absolute value. For radiating atoms, however, such elimination of the transients is not feasible. The unperturbed state is one in which one or more <u>bare</u> electrons are bound in an electrostatic potential. The transient behavior consists in the electrons' clothing themselves with virtual photons, and the non-unitary values of the $Z_\pm'$ reflect

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* In some cases of importance the barrier is so thick that decay is extremely slow, and only the level shift is of physical importance. The level shift is then customarily computed by the Rayleigh-Schrödinger perturbation formula (Section 9). The formula, however, actually diverges as a power series in g since the shifted level $E' = \mathrm{Re}\, E_\pm'$ overlaps the continuous spectrum. This mathematical situation is well known, for example, in the theory of the Stark effect. (See reference [3], p. 403 ff., and also reference [82].)

the usual renormalization problem for quantized field theories. Evidently it is not easy to define in a precise manner just exactly what constitutes an actual physical excited state. This depends on how the state was excited and can be given a rigorous definition only in terms of scattering processes. The S-matrix will be discussed below, but at this stage of our analysis the best we can do is to introduce a renormalized bare state vector:

$$|\gamma_c'\rangle = Z_+^{-\frac{1}{2}} \, |\gamma_c'\rangle . \tag{11.54}$$

We cannot, for example, allow the excited electrons first to become clothed and then look at them, because the complete clothing process requires an infinite amount of time--as indicated by the application of the operator $\bar{\mathcal{U}}(0, -\infty)$ --and by then the state will have decayed.

Using the vectors $|\gamma_c'\rangle$ one may write

$$\left|\langle\gamma_c' \,|\, \bar{\mathcal{U}}(t, 0) \,|\, \gamma_c'\rangle\right|^2 \approx e^{-\Gamma' t} \tag{11.55}$$

for times t after the transient effects have mostly settled down and before the straggling effects take over. (In practice this includes all times which are experimentally of interest.) The average lifetime of the state $|\gamma_c'\rangle$ is evidently $1/\Gamma'$, and on a statistical basis this confirms the previous interpretation of Γ' as the rate of transition out of the state.

Natural line breadth.

It is of interest to know the decay products of the state $|\gamma_c'\rangle$ after an infinite amount of time has passed. Obviously these can consist only of stable states, and hence one is led to consider the matrix elements $\langle\beta_o''|\,\bar{\mathcal{U}}(\infty, 0)\,|\gamma_c'\rangle$. With the insertion of normalization constants for the states $\langle\beta_o''|$ and use of Eqs. (6.8) and (11.17), these matrix

elements take the form

$$\left\langle \beta_-'' \middle| \gamma_c' \right\rangle = i\,\epsilon\,(Z''\,Z_+')^{-\frac{1}{2}} \left\langle \beta_o'' \middle| G_+(E'') \middle| \gamma_o' \right\rangle$$

$$= \frac{\left\langle \beta_o'' \middle| D_{c+} \middle| \gamma_o' \right\rangle}{E'' - E_+' - \Sigma_{c+}'(E)} \tag{11.56}$$

where

$$\left\langle \beta_o'' \middle| D_{c\pm} \middle| \gamma_o' \right\rangle = Z''^{-\frac{1}{2}}\, Z_\pm'^{\frac{1}{2}} \left\langle \beta_o'' \middle| D_\pm(E'') \middle| \gamma_o' \right\rangle . \tag{11.57}$$

When Γ' is small one may write approximately

$$\left| \left\langle \beta_-'' \middle| \gamma_c' \right\rangle \right|^2 \approx \frac{\left| \left\langle \beta_o'' \middle| D_{c+} \middle| \gamma_o' \right\rangle \right|^2}{(E'' - E')^2 + \frac{1}{4}\Gamma'^2} . \tag{11.58}$$

When the system H_o has only one excited state this equation may be used immediately in an analysis of the probability distribution of the final states $\left\langle \beta_o'' \right|$, and the level width Γ' is seen to have a direct interpretation as a <u>line breadth</u>. When other excited states are present, however, the analysis is not so simple since the description of important processes in which the excited states themselves act as temporary decay products is hidden in the numerator of (11.58). The most clean cut example of this is provided by the radiative decay of the hydrogen atom, for which the analysis is easily carried out in terms of diagrams:

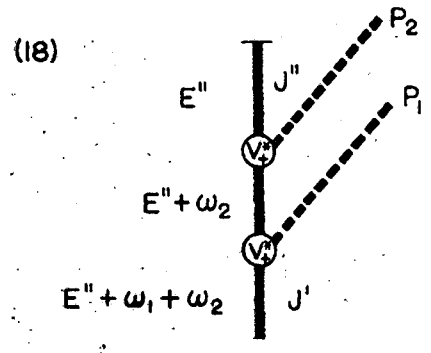
Let the initial excited state of the hydrogen atom be denoted by $\left| J' \right\rangle$, and let the final decay product be a stable state $\left| J'', \underset{\sim}{p}_1, \underset{\sim}{p}_2 \right\rangle$ in which the atom is in a ground state (denoted by J'') and <u>two</u> real photons are present having momenta $\underset{\sim}{p}_1$ and $\underset{\sim}{p}_2$ respectively. (For simplicity we omit labels referring to the polarization of the photons.) The most

important irreducible diagram leading to such a final state, pictured in Fig. 18, involves an intermediate state in which only one real photon is present. (Lines representing the external impressed electrostatic field of the proton have not been included in the figure.) Since the momentum of the intermediate photon may be either $\underset{\sim}{p}_1$ or $\underset{\sim}{p}_2$ the contribution of this diagram to expression (11.56) is

$$e^2(Z_2'' Z_3^2)^{\frac{1}{2}} Z_{2+}'^{-\frac{1}{2}} \Big\langle J'' \Big| \Big[V_+^*(\underset{\sim}{p}_2)S_+(E''+\omega_2)V_+^*(\underset{\sim}{p}_1)S_+(E''+\omega_1+\omega_2) + V_+^*(\underset{\sim}{p}_1)S_+(E''+\omega_1)V_+^*(\underset{\sim}{p}_2)S_+(E''+\omega_1+\omega_2)\Big] \Big| J' \Big\rangle \tag{11.59}$$

where the notation is obvious: E'' is the energy of the electron in the state J'', including the electrodynamic correction, ω_1 and ω_2 are the photon energies, Z_2'' is the electron normalization constant for the final state, Z_{2+}' is that for the initial state, Z_3 is the usual photon normalization constant, e is the bare electronic charge, $V_+^*(\underset{\sim}{p})$ is the modified vertex operator for the emission of a photon of momentum $\underset{\sim}{p}$, and $S_+(E)$ is the modified electron propagation function.

In the present example, with an impressed electrostatic field, the classification of electron states based on the bound state labels J possesses none of the relativistic invariance properties of the momentum classification used for free particle problems. The electron-photon coupling is therefore not "symmetric" in the sense explained in section 10, and the propagation function $S_+(E)$ is here not diagonal in the bound state labels. Eq. (11.17) shows, however, that the off-diagonal elements are of higher order in the electronic charge than the diagonal elements, and therefore one may to good



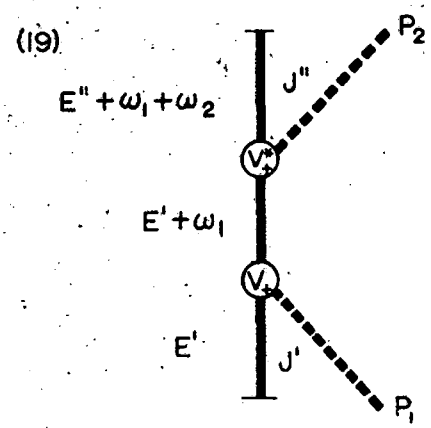


FIG. 18 DIAGRAM FOR TWO-PHOTON DECAY
FIG. 19 DIAGRAM FOR RESONANCE SCATTERING

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approximation consider only the latter.* With the absorption of the normalization constants into the definition of the renormalized charge,** propagation function and vertex operator,** and with the replacement of the latter (as a second approximation) by the simple unmodified vertex operator V_o^*, expression (11.59) then takes the form

$$e_c^2 \sum{}''' \left[\frac{\langle J'' | V_o^*(\underset{\sim}{p}_2) | \alpha''' \rangle \langle \alpha''' | V_o^*(\underset{\sim}{p}_1) | J' \rangle}{E'' + \omega_2 - E_+''' - \Sigma_{c+}'''(E'' + \omega_2)} \right. \tag{11.60}$$

$$\left. + \frac{\langle J'' | V_o^*(\underset{\sim}{p}_1) | \alpha''' \rangle \langle \alpha''' | V_o^*(\underset{\sim}{p}_2) | J' \rangle}{E'' + \omega_1 - E_+''' - \Sigma_{c+}'''(E'' + \omega_1)} \right]$$

$$\times \frac{1}{E'' + \omega_1 + \omega_2 - E_+' - \Sigma_{c+}'(E'' + \omega_1 + \omega_2)} ,$$

the labels α''' referring to the intermediate electronic states. Squaring the absolute value of this expression and neglecting the renormalized self-energy function Σ_{c+}, one gets for the two-photon decay distribution

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* For estimates of the errors introduced by this and subsequent approximations see reference [90].

** $V_c = Z_1 V$ and $e_c = Z_1^{-1} Z_2 Z_3^{\frac{1}{2}} e$ where Z_2 is the renormalization constant for the free electron. Z_{2+}' and Z_2'' are "approximately" equal to Z_2.

$$P(J'', \underset{\sim}{p}_1, \underset{\sim}{p}_2 \mid J')$$

$$\approx \frac{e_c^4}{(E'' + \omega_1 + \omega_2 - E')^2 + \frac{1}{4}\Gamma'^2} \sum^{''',''''} \left[\frac{\langle J'' | V_o^*(\underset{\sim}{p}_2) | \alpha''' \rangle \langle \alpha''' | V_o^*(\underset{\sim}{p}_1) | J' \rangle}{E'' + \omega_2 - E''' + \frac{1}{2} i \Gamma'''} \right.$$

$$\left. + \frac{\langle J'' | V_o^*(\underset{\sim}{p}_1) | \alpha''' \rangle \langle \alpha''' | V_o^*(\underset{\sim}{p}_2) | J' \rangle}{E'' + \omega_1 - E''' + \frac{1}{2} i \Gamma'''} \right]$$

$$\times \left[\frac{\langle J'' | V_o^*(\underset{\sim}{p}_2) | \alpha'''' \rangle^* \langle \alpha'''' | V_o^*(\underset{\sim}{p}_1) | J' \rangle^*}{E'' + \omega_2 - E'''' - \frac{1}{2} i \Gamma''''} \right.$$

$$\left. + \frac{\langle J'' | V_o^*(\underset{\sim}{p}_1) | \alpha'''' \rangle^* \langle \alpha'''' | V_o^*(\underset{\sim}{p}_2) | J' \rangle^*}{E'' + \omega_1 - E'''' - \frac{1}{2} i \Gamma''''} \right] \tag{11.61}$$

In practice (e.g. ordinary spectroscopic work) the two photons are never observed simultaneously. The quantity of primary physical interest is therefore

$$P_2(J'', \underset{\sim}{p}_1 \mid J') = \sum_{p_2} P(J'', \underset{\sim}{p}_1, \underset{\sim}{p}_2 \mid J') \tag{11.62}$$

which is the total probability of finding one of the photons in the state $\underset{\sim}{p}_1$ no matter what state the other photon may be in. This probability distribution, when integrated over the solid angle $\underset{\sim}{\Omega}_1$, gives immediately the line structure generated by two-step decay of the excited state $| J' \rangle$.

It is of course does not include the direct one-step line structure which is given by

$$P_1(J'', \underset{\sim}{p_1} \mid J') \approx \frac{e_c^2 \left| \left\langle J'' \middle| V_o^*(\underset{\sim}{p_1}) \middle| J' \right\rangle \right|^2}{\left[\omega_1 - (E' - E'')\right]^2 + \frac{1}{4}\Gamma'^2} . \tag{11.63}$$

In the most general cases expression (11.61) may lead to very complicated line structures. We shall consider only the simple standard case in which the level widths Γ''' are all very small compared to the level separations $E' - E'''$, $E''' - E''$ and in which none of the discrete lines, to which these separations give rise, overlap one another. First of all, under these circumstances the cross terms in the product under the summation in (11.61) are easily seen to give a negligible contribution. Since Γ' is small the factor out in front is essentially a delta function, so that one may set $\omega_2 = E' - E'' - \omega_1$ in these terms, which then become

$$- \sum^{''',''''} \left\{ \frac{\left\langle J'' \middle| V_o^*(\underset{\sim}{p_2}) \middle| \alpha''' \right\rangle \left\langle \alpha''' \middle| V_o^*(\underset{\sim}{p_1}) \middle| J' \right\rangle \left\langle J' \middle| V_o(\underset{\sim}{p_2}) \middle| \alpha'''' \right\rangle \left\langle \alpha'''' \middle| V_o(\underset{\sim}{p_1}) \middle| J'' \right\rangle}{\left[\omega_1 - (E' - E''') - \frac{1}{2} i\Gamma'''\right]\left[\omega_1 - (E'''' - E'') - \frac{1}{2} i\Gamma''''\right]} \right.$$

$$\left. + \text{ complex conjugate} \right\} . \tag{11.64}$$

Since $\omega_1 > 0$ and since $|J'\rangle$ and $|J''\rangle$ are bound states with $E' > E''$, the factors in the denominator of (11.64) become small only for states $|\alpha'''\rangle$ and $|\alpha''''\rangle$ which are bound, with $E' > E'''$ and $E'''' > E''$. Both factors cannot become small simultaneously, however, owing to the assumption that the discrete lines do not overlap; therefore (11.64) always has values negligible compared to the peak values of the other terms to be discussed next.

The terms in the product which involve only ω_1 refer to a physical situation in which the unobserved photon of momentum $\underset{\sim}{p}_2$ is emitted first, followed by direct decay of the resulting intermediate excited state $|\alpha'''\rangle$ to the ground state. Here the assumed non-overlap of the discrete lines effectively reduces the double summation to a single summation, namely

$$\sum{}''' \frac{\left|\langle J'' | V_o^*(\underset{\sim}{p}_1) | \alpha'''\rangle\right|^2 \left|\langle \alpha''' | V_o^*(\underset{\sim}{p}_2) | J'\rangle\right|^2}{\left[\omega_1 - (E''' - E'')\right]^2 + \frac{1}{4}\Gamma'''^2} . \tag{11.65}$$

The delta function character of the factor in front in (11.61), combined with the fact that $\omega_2 > 0$,* leads to the requirement $\omega_1 < E' - E''$. The summation in (11.65) therefore need be carried out only over bound states $|J'''\rangle$ with $E'' < E''' < E'$. The validity of the omission of the cross terms in the product in (11.61) and of the off-diagonal terms in the double summation expresses an important physical fact, namely that the successive emission processes for the two photons are statistically independent of one another.

There remain the terms involving ω_2 only. Here again the double summation reduces effectively to a single summation, but the integration over ω_2 which occurs in (11.62) is now more complicated than before. The smallness of the level widths, however, allows the integration to be simplified. First of all, $V_o^*(\underset{\sim}{p}_2)$ will generally have negligible

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* This follows from the fact that the electrodynamic vertex operator $V_o^*(\underset{\sim}{p})$ vanishes as $\underset{\sim}{p} \rightarrow 0$.

variation across each peak of the function (11.61) and may therefore be regarded as a constant (evaluated at the peak) in the ω_2 integration. Secondly, if the summation is restricted in advance to bound states $|J'''\rangle$ with $E'' < E''' < E'$, then negligible error is introduced if the range of integration is altered from $(0, \infty)$ to $(-\infty, \infty)$. Hence, using the integral identity

$$\int_{-\infty}^{\infty} \frac{dx}{\left[(x-a)^2 + c^2\right]\left[(x-b)^2 + d^2\right]} = \frac{\pi}{cd} \frac{c+d}{(a-b)^2 + (c+d)^2} , \tag{11.66}$$

for $c, d > 0$, and the fact that $p_1 = \omega_1$ for photons, one gets

$$P_2(J'', \underset{\sim}{p}_1 | J') \approx e_c^4 \left(\frac{L}{2\pi}\right)^3 \frac{2\pi}{\Gamma'} \sum_{E'' < E''' < E'}''' \left[\frac{\Gamma' + \Gamma'''}{\Gamma'''} \frac{\left|\langle J''' | V_o^*(\underset{\sim}{p}_1) | J' \rangle\right|^2 (E''' - E'')^2}{\left[\omega_1 - (E' - E''')\right]^2 + \frac{1}{4}(\Gamma' + \Gamma''')^2} \right.$$

$$\times \int \left|\langle J'' | V_o^*((E''' - E'')\underset{\sim}{\Omega}) | J''' \rangle\right|^2 d^2\underset{\sim}{\Omega}$$

$$+ \frac{\left|\langle J'' | V_o^*(\underset{\sim}{p}_1) | J''' \rangle\right|^2 (E' - E''')^2}{\left[\omega_1 - (E''' - E'')\right]^2 + \frac{1}{4}\Gamma'''^2}$$

$$\left. \times \int \left|\langle J''' | V_o^*((E' - E''')\underset{\sim}{\Omega}) | J' \rangle\right|^2 d^2\underset{\sim}{\Omega} \right] . \tag{11.67}$$

The point to which one may now call attention is the well known fact that the breadth of an emission line resulting from an atomic transition between two <u>excited</u> states (e.g. $|J'\rangle$ and $|J'''\rangle$) is equal to the <u>sum</u> $(\Gamma + \Gamma''')$

of the widths of the individual levels. In fact, the simpler result for the transition from an excited state to a ground state may be regarded as a special case, in which the width of the lower level vanishes. The sum in question is known as the natural line breadth. For atomic systems the experimental arrangement is usually such that the natural line breadth is completely non-measurable because of the effects of collision and Doppler broadening. For nuclear transitions, however, the natural line breadth can be quite significant, and the equations written above may have useful applicability, subject to the restrictive assumptions mentioned at the outset. The modification of these equations for cases in which the emitted particles are other than photons is obvious and straightforward.

The consistency of the approximations which have been made in the above equations can be readily checked. One needs for this purpose an approximate expression for the level widths. Eq. (11.39) may serve as a basis for discussion. Unfortunately this equation is not easily written in a closed form involving renormalized quantities only. Therefore one must fall back on a power series expansion in the renormalized electronic charge e_c and show that all divergences cancel to any given order. We make no attempt to carry out this program here, but rest content with the lowest order result. Remembering that $Z' = 1 - O(e_c^2)$ and $e^2 = e_c^2 + O(e_c^4)$, we find

$$\Gamma' \approx 2\pi e_c^2 \sum_{J'',\underset{\sim}{p}} \delta(E'' + \omega - E') \left| \langle J'' | V_o^*(\underset{\sim}{p}) | J' \rangle \right|^2$$

$$= \sum_{E'' < E'}'' \Gamma(J'' | J') \tag{11.68}$$

where

$$\Gamma(J'' | J') = 2\pi e_c^2 (L/2\pi)^3 (E' - E'')^2 \int \left| \langle J'' | V_o^*((E' - E'')\underset{\sim}{\Omega}) | J' \rangle \right|^2 d^2\underset{\sim}{\Omega}. \tag{11.69}$$

If one sets

$$\Gamma(J'' \mid J') \equiv 0 \qquad \text{for } E'' \geqslant E' \ , \tag{11.70}$$

then the instructions "$E'' < E'$" may be omitted in (11.68).

If one removes the angular dependence of the functions $P_1(J'', \underset{\sim}{p} \mid J')$ and $P_2(J'', \underset{\sim}{p} \mid J')$ by defining

$$P_n(J'', \omega \mid J') = (L/2\pi)^3 \, \omega^2 \int P_n(J'', \omega \underset{\sim}{\Omega} \mid J') d^2\underset{\sim}{\Omega}, \tag{11.71}$$

$$\int_0^\infty P_n(J'', \omega \mid J') d\omega = \sum_{\underset{\sim}{p}} P_n(J'', \underset{\sim}{p} \mid J') \ , \qquad n = 1, 2 \ldots , \tag{11.72}$$

then one may write

$$P_1(J'', \omega \mid J') \approx \frac{1}{2\pi} \frac{\Gamma(J'' \mid J')}{\left[\omega - (E' - E'')\right]^2 + \frac{1}{4}\Gamma'^2} \tag{11.73}$$

$$P_2(J'', \omega \mid J') \approx \frac{1}{2\pi} \sum{}''' \frac{\Gamma(J'' \mid J''') \Gamma(J''' \mid J')}{\Gamma' \, \Gamma'''}$$

$$\times \left[\frac{\Gamma' + \Gamma'''}{\left[\omega - (E' - E''')\right]^2 + \frac{1}{4}(\Gamma' + \Gamma''')^2} + \frac{\Gamma'''}{\left[\omega - (E''' - E'')\right]^2 + \frac{1}{4}\Gamma'''^2} \right] \tag{11.74}$$

Similarly, the line-structure functions for decay processes involving three or more steps are given, as one may easily show, by

$$P_3(J'', \omega \mid J') \approx \frac{1}{2\pi} \sum{}'''^{,''''} \frac{\Gamma(J'' \mid J'''') \Gamma(J'''' \mid J''') \Gamma(J''' \mid J')}{\Gamma' \, \Gamma''' \, \Gamma''''}$$

$$\left[\frac{\Gamma' + \Gamma'''}{\left[\omega - (E' - E''')\right]^2 + \frac{1}{4}(\Gamma' + \Gamma''')^2} + \frac{\Gamma''' + \Gamma''''}{\left[\omega - (E''' - E'''')\right]^2 + \frac{1}{4}(\Gamma''' + \Gamma'''')^2} \right.$$

$$\left. + \frac{\Gamma''''}{\left[\omega - (E'''' - E'')\right]^2 + \frac{1}{4}\Gamma''''^2} \right], \tag{11.75}$$

and so on. Since a permutation of the $n - 1$ unobserved photons does not change the final state one must remember to define

$$P_n(J'', \underset{\sim}{p}_1 | J') = \left[(n-1)!\right]^{-1} \sum_{\underset{\sim}{p}_2 \cdots \underset{\sim}{p}_n} P(J'', \underset{\sim}{p}_1, \underset{\sim}{p}_2 \cdots \underset{\sim}{p}_n | J'). \tag{11.76}$$

The consistency of the various approximations may now be verified by invoking the condition that $|J'\rangle$, being an unstable state, must have unit probability for decaying. This probability may be expressed, however, as the sum of the probabilities for all the various single and multi-step decay processes. Taking into account photon indistinguishability one should therefore have

$$1 = \sum{}'' \sum_n n^{-1} \int P_n(J'', \omega | J') d\omega$$

$$\approx \sum{}'' \left[\frac{\Gamma(J'' | J')}{\Gamma'} + \sum{}''' \frac{\Gamma(J'' | J''') \Gamma(J''' | J')}{\Gamma' \Gamma'''} + \sum{}^{''',''''} \frac{\Gamma(J'' | J'''') \Gamma(J'''' | J''') \Gamma(J''' | J')}{\Gamma' \Gamma''' \Gamma''''} + \cdots \right] \tag{11.77}$$

where the summation $\sum''$ is carried out only over the <u>stable</u> bound states $|J''\rangle$. Equation (11.77) indeed holds <u>exactly</u>, as may be proved simply by induction from Eq. (11.68) together with use of the fact that $\Gamma(J'''' | J''')$ vanishes for all $|J''''\rangle$ if $|J'''\rangle$ is a stable state.

If we return now to the exact equation (11.56) we appear, at first sight, to have been led to a contradiction. For what we seem to be computing in (11.77) is the square of the absolute value of $\langle \beta_-'' | \gamma_c' \rangle$ summed over all final states $|\beta_o''\rangle$. But since the vectors $|\beta_-''\rangle$ form a

complete set we must have, in virtue of the renormalization (11.54),

$$\sum{}'' \left|\langle \beta_-'' | \gamma_c' \rangle\right|^2 = \left|z_+'\right|^{-1} . \tag{11.78}$$

The discrepancy lies in the summation over intermediate and high energy photons. It is to be remembered that the approximate forms (11.63), (11.67), (11.73), (11.74), (11.75), etc. for the line-structure functions are valid only in the vicinity of the peaks. The high-energy tails as well as the "valleys" of these functions are incorrectly given by the approximate forms owing to the neglect of 1) the self-energy functions which appear in the denominators of Eq. (11.60), 2) the cross terms, and 3) the summations over the continuum electronic levels (as well as bound levels) having energy greater than E'. To be sure, even the true values of these functions in the tail and valley regions are negligible compared to the peak values, but their deviation from the values of the approximate formulae is significant when integrations are performed and is, in fact, just sufficient to account for the discrepancy between Eqs. (11.77) and (11.78).

It is evident that the "approximate" expressions have a closer relation to physical reality than the exact ones. Neglect of the self-energy functions, continuum levels, etc. must correspond in some sense to ignoring the "clothing process" of the bare electron, which is unobservable anyway.

The S-matrix.

In Sec. 10 we showed how a renormalized S-matrix could be defined within the context of a simple field theory with symmetric coupling. We now must do this for the general case. Eqs. (7.23) and (7.25) provide a convenient starting point, if rewritten in the forms

$$\delta_{E''E'} \text{ Sing } \langle \beta_o'' | \beta_\pm' \rangle = Z'^{\frac{1}{2}} \delta(\beta_o'', \beta_o') \quad , \tag{11.79}$$

$$\delta_{E''E'} \langle \beta_o'' | \text{ Sing } \mathcal{R}_\pm | \beta_o' \rangle = \pm i\epsilon (Z' - 1) \delta(\beta_o'', \beta_o') \quad . \tag{11.80}$$

Here only the stable states $|\beta_o'\rangle$ are considered, and the symbol "Sing" has been inserted in (11.79) so as to generalize Eq. (7.23) which was valid only for discrete-spectrum (bound state) theory. One will recall that the symbol "Sing" separates out that part of a given expression which is independent of the dimensions L of the normalizing box. Thus for example, if the free states of the simple system described by Fig. 17 are involved then Sing$\langle \beta_o'' | \beta_\pm' \rangle$ vanishes except when $\beta_o'' = \beta_o'$ since $\langle \beta_o'' | \beta_\pm' \rangle$ is of order L^{-N} for $\beta_o'' \neq \beta_o'$. (In this example, of course, $Z' = 1$ for the free states.) If stable bound states (if any) are involved then $\langle \beta_o'' | \beta_\pm' \rangle$ has no nonsingular part, and the diagonal character of $\delta_{E''E'} \langle \beta_o'' | \beta_\pm' \rangle$ depends on the nonremovable nature of any degeneracy which persists as the perturbation is switched on. For complex systems involving interacting fields the singular part of $\delta_{E''E'} \langle \beta_o'' | \beta_\pm' \rangle$ can always, just as in the example of the preceding section, be correlated pictorially with diagrams in which the individual real particles involved undergo self-energy interactions with virtual quanta but do not interact with each other. Again the diagonal character of this singular part depends on the nonremovability of any persistent degeneracy.

In the preceding section we have seen that the correct definition of the renormalized S-matrix depends on a careful evaluation of the "derivative term" in Eq. (7.40). Only the singular part of this term contributes in the limit $\epsilon \to 0$ and therefore all that is needed is a straightforward generalization of Eq. (10.89), namely

$$\delta_{E''E'} \text{ Sing } \langle \beta_o'' | \partial \mathcal{R}_\pm(E')/\partial E' | \beta_o' \rangle = (Z' - 1) \delta(\beta_o'', \beta_o') \quad . \tag{11.81}$$

This equation, in fact, follows from Eq. (10.81) which may be written in the matrix form

$$\langle \beta_o'' | \mathcal{R}_\pm(E) | \beta_o' \rangle$$

$$= (E - E'' \pm i\epsilon)(E - E' \pm i\epsilon) \sum{}''' \frac{\langle \beta_o'' | \beta_\pm''' \rangle \langle \beta_\pm''' | \beta_o' \rangle}{E - E''' \pm i\epsilon} - (E - E' \pm i\epsilon)\, \delta(\beta_o'', \beta_o') \tag{11.82}$$

Differentiation with respect to E gives [32]

$$\delta_{E''E'} \langle \beta_o'' | \partial \mathcal{R}_\pm(E')/\partial E' | \beta_o' \rangle$$

$$= \delta_{E''E'} \sum{}''' \left[1 - \frac{(E' - E''')(E'' - E''')}{(E' - E''' \pm i\epsilon)^2} \right] \langle \beta_o'' | \beta_\pm''' \rangle \langle \beta_\pm''' | \beta_o' \rangle - \delta(\beta_o'', \beta_o') , \tag{11.83}$$

the singular part of which leads, via (11.79), to Eq. (11.81).

Remembering that

$$Z'^{\frac{1}{2}} | \beta_\pm' \rangle = \left[1 + G_{o\pm}(E') \mathcal{R}_\pm(E') \right] | \beta_o' \rangle , \tag{11.84}$$

repeating the derivation of Eq. (7.40), and using Eqs. (11.80, 81) and the identity $\delta(\beta_o'', \beta_o')\delta(E'' - E') = (\pi\epsilon)^{-1}\delta(\beta_o'', \beta_o')$, one finds that the renormalized S-matrix is given by [32]

$$\langle \beta_o'' | S_c^{\pm 1} | \beta_o' \rangle \equiv \langle \beta_\mp'' | \beta_\pm' \rangle$$

$$= (Z''Z')^{-\frac{1}{2}} \Big\{ \left[1 \mp 2i\epsilon^{-1}(\pm i\epsilon \mp \tfrac{1}{2}i\epsilon)(Z' - 1) \right] \delta(\beta_o'', \beta_o')$$

$$\mp 2\pi i\, \delta(E'' - E') \langle \beta_o'' | R_\pm | \beta_o' \rangle \Big\}$$

$$= \delta(\beta_0'', \beta_0') \mp i \left\langle \beta_0'' \middle| \underset{\sim}{R}_{c\pm} \middle| \beta_0' \right\rangle , \tag{11.85}$$

where

$$\left\langle \beta_0'' \middle| \underset{\sim}{R}_{c\pm} \middle| \beta_0' \right\rangle = (Z'' Z')^{-\frac{1}{2}} \left\langle \beta_0'' \middle| \underset{\sim}{R}_{\pm} \middle| \beta_0' \right\rangle , \tag{11.86}$$

$R_{\pm}$ being, as one will recall, the "remainder" of $\mathcal{R}_{\pm}$ after the singular part has been subtracted. $\underset{\sim}{R}_{c\pm}$ is the renormalized transition operator.

Resonance scattering.

We shall illustrate the use of Eq. (11.86) with the hydrogen atom previously considered. Suppose the unexcited atom scatters a photon of momentum $\underset{\sim}{p}_1$ so that the system undergoes a transition from a state $|J', \underset{\sim}{p}_1\rangle$ to a state $|J'', \underset{\sim}{p}_2\rangle$, both $|J'\rangle$ and $|J''\rangle$ being ground states (possibly identical) of the atom. The irreducible scattering diagram which gives the principal contribution to this process is pictured in Fig. 19, and one may write

$$\begin{aligned}
&\left\langle J'', \underset{\sim}{p}_2 \middle| \underset{\sim}{R}_{c+} \middle| J', \underset{\sim}{p}_1 \right\rangle \\
&\approx 2\pi\, \delta(E'' + \omega_2 - E' - \omega_1)\, e^2 (Z_2'' Z_2' Z_3^2)^{\frac{1}{2}} \left\langle J'' \middle| V_+^*(\underset{\sim}{p}_2) S_+(E' + \omega_1) V_+(\underset{\sim}{p}_1) \middle| J' \right\rangle \\
&\approx 2\pi\, \delta(E'' + \omega_2 - E' - \omega_1)\, e_c^2 \sum{}''' \frac{\left\langle J'' \middle| V_c^*(\underset{\sim}{p}_2) \middle| \alpha''' \right\rangle \left\langle \alpha''' \middle| V_c(\underset{\sim}{p}_1) \middle| J' \right\rangle}{E' + \omega_1 - E_+''' - \sum_{c+}''(E' + \omega_1)} .
\end{aligned} \tag{11.87}$$

We shall consider only photons having energies less than that required to ionize the atom. If accuracy is desired only near the resonance peaks the summation in Eq. (11.87) need then be carried out only over the bound atomic states $|J'''\rangle$. Moreover, when the square of the absolute value of this expression is taken, the resulting double summation may be reduced to a single

summation in the familiar manner, and, using Eq. (8.12), one may write the transition rate as

$$R(J'', \underset{\sim}{p}_2 \,|\, J', \underset{\sim}{p}_1)$$

$$\approx 2\pi\,\delta(E'' + \omega_2 - E' - \omega_1)\, e_c^{\,4} \sum^{'''} \frac{\left|\left\langle J'' \middle| V_c^{\,*}(\underset{\sim}{p}_2) \middle| J''' \right\rangle\right|^2 \left|\left\langle J''' \middle| V_o(\underset{\sim}{p}_1) \middle| J' \right\rangle\right|^2}{\left[\omega_1 - (E''' - E')\right]^2 + \frac{1}{4}\Gamma'''^2} \tag{11.88}$$

from which the angular scattering cross section may immediately be obtained. Expression (11.88) shows the well known phenomenon of <u>resonance scattering</u> in which the cross section becomes anomalously large when the initial photon energy ω_1 has a value in the neighborhood of one of the level separations $E''' - E'$.

As a check on the consistency of our approximations in the present case we may make use of the probability conservation theorem expressed by Eq. (8.33). In order to apply this theorem, however, we need matrix elements of the transition operator which describe processes in which more than one photon is present in the final state. Thus we compute

$$\left\langle J'', \underset{\sim}{p}_2, \underset{\sim}{p}_3 \middle| \underset{\sim}{R}_{c+} \middle| J', \underset{\sim}{p}_1 \right\rangle \approx 2\pi\,\delta(E'' + \omega_2 + \omega_3 - E' - \omega_1)\, e^3 (Z_2'' Z_2 Z_1')^{\frac{1}{2}}$$

$$\times \left\langle J'' \middle| \left[V_+^{\,*}(\underset{\sim}{p}_3) S_+(E' + \omega_1 - \omega_2) V_+^{\,*}(\underset{\sim}{p}_2) S_+(E' + \omega_1) V_+(\underset{\sim}{p}_1) \right.\right.$$

$$\left.\left. + \; V_+(\underset{\sim}{p}_2) S_+(E' + \omega_1 - \omega_3) V_+^{\,*}(\underset{\sim}{p}_3) S_+(E' + \omega_1) V_+(\underset{\sim}{p}_1) \right] \middle| J' \right\rangle$$

$$\approx 2\pi\,\delta(E'' + \omega_2 + \omega_3 - E' - \omega_1)\, e_c^{\,3} \sum^{''',''''}$$

$$\left\{ \frac{\left\langle J'' \middle| V_o^{\,*}(\underset{\sim}{p}_3) \middle| \alpha'''' \right\rangle \left\langle \alpha'''' \middle| V_o^{\,*}(\underset{\sim}{p}_2) \middle| \alpha''' \right\rangle \left\langle \alpha''' \middle| V_c(\underset{\sim}{p}_1) \middle| J' \right\rangle}{\left[E' + \omega_1 - \omega_2 - E_+''' - \Sigma_{c+}''''(E' + \omega_1 - \omega_2)\right]\left[E' + \omega_1 - E_+''' - \Sigma_{c+}'''(E' + \omega_1)\right]} + \widetilde{2} \right\} \tag{11.89}$$

$$R(J'', \underset{\sim}{p}_2, \underset{\sim}{p}_3 | J', \underset{\sim}{p}_1) \approx 2\pi\,\delta(E'' + \omega_2 + \omega_3 - E' - \omega_1) e_c^6 \sum^{''',''''}$$

$$\left\{ \frac{\left|\left\langle J'' \middle| V_o^*(\underset{\sim}{p}_3) \middle| J'''' \right\rangle\right|^2 \left|\left\langle J'''' \middle| V_o^*(\underset{\sim}{p}_2) \middle| J''' \right\rangle\right|^2 \left|\left\langle J''' \middle| V_o(\underset{\sim}{p}_1) \middle| J' \right\rangle\right|^2}{\left[(E' + \omega_1 - \omega_2 - E'''')^2 + \frac{1}{4}\Gamma''''^2\right]\left[(E' + \omega_1 - E''')^2 + \frac{1}{4}\Gamma'''^2\right]} + \widetilde{23} \right\}$$

(11.90)

and so on. Here the notation $\widetilde{23}$ indicates that the same expression is to be repeated but with the two final photons interchanged.

Eq. (8.33) may, for the one-initial-photon case, be written in the form

$$-2\,\mathrm{Im}\left\langle J', \underset{\sim}{p}_1 \middle| R_{c+} \middle| J', \underset{\sim}{p}_1 \right\rangle$$

$$= \sum{}'' \left[\sum_{\underset{\sim}{p}_2} R(J'', \underset{\sim}{p}_2 | J', \underset{\sim}{p}_1) + \tfrac{1}{2} \sum_{\underset{\sim}{p}_2, \underset{\sim}{p}_3} R(J'', \underset{\sim}{p}_2, \underset{\sim}{p}_3 | J', \underset{\sim}{p}_1) + \cdots \right]$$

$$\approx \sum{}''' \left\{ \sum{}'' \left[\Gamma(J'' | J''') + \sum{}'''' \frac{\Gamma(J'' | J'''')\Gamma(J'''' | J''')}{\Gamma''''} + \cdots \right] \right.$$

$$\left. \times\; e_c^2 \frac{\left|\left\langle J''' \middle| V_o(\underset{\sim}{p}_1) \middle| J' \right\rangle\right|^2}{\left[\omega_1 - (E''' - E')\right]^2 + \frac{1}{4}\Gamma'''^2} \right\}$$

(11.91)

where $\sum''$ denotes a summation only over the stable bound states $|J''\rangle$. On the other hand, from Eq. (11.87),

$$-2\,\mathrm{Im}\left\langle J', \underset{\sim}{p}_1 \middle| R_{c+} \middle| J', \underset{\sim}{p}_1 \right\rangle \approx e_c^2 \sum{}''' \Gamma''' \frac{\left|\left\langle J''' \middle| V_o(\underset{\sim}{p}_1) \middle| J' \right\rangle\right|^2}{\left[\omega_1 - (E''' - E')\right]^2 + \frac{1}{4}\Gamma'''^2}$$

(11.92)

The consistency is now evident since, from Eq. (11.77), the right-hand sides of Eqs. (11.93, 92) are equal. Conservation of probability may be similarly

verified for the many-initial-photon cases.

The phenomenon of resonance scattering may also occur for simple systems of the type described by Fig. 17. Here there is no renormalization problem and using Eq. (7.3), one may write directly

$$\begin{aligned}\langle \zeta_0''' | R_+ | \zeta_0'' \rangle &= \langle \zeta_0''' | [H_1 + H_1 G_+(E'') H_1] | \zeta_0'' \rangle \\ &\approx \langle \zeta_0''' | H_1 | J_0' \rangle \langle J_0' | G_+(E'') | J_0' \rangle \langle J_0' | H_1 | \zeta_0'' \rangle \\ &= Z_+' \frac{\langle \zeta_0''' | B | J_0' \rangle \langle J_0' | B | \zeta_0'' \rangle}{E'' - E_+' - \Sigma_{c+}'(E'')} ,\end{aligned} \tag{11.93}$$

and, since one has $Z_+' \approx 1$ if B is properly chosen, the transition rate in the neighborhood of the resonance peak is given by

$$R(\zeta_0''' | \zeta_0'') \approx 2\pi \delta(E''' - E'') \frac{|\langle \zeta_0''' | B | J_0' \rangle|^2 \, |\langle J_0' | B | \zeta_0'' \rangle|^2}{(E'' - E')^2 + \frac{1}{4}\Gamma'^2} \tag{11.94}$$

The probability conservation theorem has here the form

$$-2 \operatorname{Im} \langle \zeta_0'' | R_+ | \zeta_0'' \rangle = \sum{}''' R(\zeta_0''' | \zeta_0'') , \tag{11.95}$$

and the consistency of the approximations made in Eqs. (11.93) and (11.94) follows from the equations

$$-2 \operatorname{Im} \langle \zeta_0'' | R_+ | \zeta_0'' \rangle \approx \Gamma' \frac{|\langle J_0' | B | \zeta_0'' \rangle|^2}{(E'' - E')^2 + \frac{1}{4}\Gamma'^2} , \tag{11.96}$$

$$\Gamma' \approx 2\pi \sum{}''' \delta(E''' - E') \, |\langle \zeta_0''' | B | J_0' \rangle|^2 . \tag{11.97}$$

<u>The excitation process.</u>

The S-matrix having been properly defined, we are now in a position to give an acceptable mathematical treatment of the excitation of a given

unstable state by means of incident particles. We shall restrict the discussion to the context of hydrogen-atom-plus-radiation, so that the incident particles will be photons, but the conclusions will be quite general.

Suppose the atom is immersed in an isotropic "bath" of nearly monochromatic radiation. The individual photons constituting the bath will be scattered by the atom and produce other photons having a distribution given by

$$D(J'', \underset{\sim}{p}_2) = \sum_{\underset{\sim}{p}_1} R(J'', \underset{\sim}{p}_2 \,|\, J', \underset{\sim}{p}_1)\, I(\omega_1) , \tag{11.98}$$

$$D(J'', \underset{\sim}{p}_2, \underset{\sim}{p}_3) = \sum_{\underset{\sim}{p}_1} R(J'', \underset{\sim}{p}_2, \underset{\sim}{p}_3 \,|\, J', \underset{\sim}{p}_1)\, I(\omega_1), \text{ etc.,} \tag{11.99}$$

where $I(\omega)$ is a peaked function which characterizes the radiation bath. Let us assume that $I(\omega)$, which may be called the <u>excitation function</u>, 1) is peaked around the energy value $\omega = E''' - E'$, 2) does not sensibly overlap energy values corresponding to any of the other level separations, and 3) has a width larger than the level width Γ''' so that it is essentially constant in the range $E''' - E' - \Gamma'''$ to $E''' - E' + \Gamma'''$. Then, inserting Eqs. (11.88) and (11.90) into Eqs. (11.98, 99), and using Eqs. (11.61) and (11.63), we easily obtain

$$D(J'', \underset{\sim}{p}_2) \approx P_1(J'', \underset{\sim}{p}_2 \,|\, J''')\Gamma(J''' \,|\, J')\, I(E''' - E') , \tag{10.100}$$

$$D(J'', \underset{\sim}{p}_2, \underset{\sim}{p}_3) \approx P(J'', \underset{\sim}{p}_2, \underset{\sim}{p}_3 \,|\, J''')\Gamma(J''' \,|\, J')I(E''' - E') , \text{ etc.,} \tag{10.101}$$

these formulae being valid in the peak regions.

The distribution of scattered photons is seen to be directly proportional to the simple decay distribution which we have already calculated. The physical interpretation is obvious. The radiation bath excites the atom

from the ground state $|J'\rangle$ to the unstable state $|J'''\rangle$, and then the atom undergoes a subsequent spontaneous decay. The "scattering" is essentially <u>incoherent</u>, at least in the peak regions, since the emission process, described by the P-functions, is statistically independent of the absorption process, described by the factors $\Gamma(J'''|J')\, I(E''' - E')$.

When one speaks of a system's being brought into an excited state one is speaking, according to customary terminology, about a state which is well defined in itself and independent of the precise details of the excitation process. It is important to note, therefore, that the energy spread in the radiation bath must be greater than Γ''' in order that the bath be a true <u>excitant</u>. For if the width of $I(\omega)$ becomes less than Γ''' then, because energy is conserved under a collision, the distribution of scattered photons will begin to depend on the shape of $I(\omega)$ instead of following the natural line shape, which simply means that the scattering will no longer be incoherent.

12. PROBLEMS INVOLVING SEVERAL PERTURBATIONS

Introduction.

In many problems of great practical importance it is convenient to split a total perturbation into several parts which may be considered separately or in various combinations. This circumstance gives rise to a number of further natural developments of the operator formalism, to which we now turn our attention.

The total Hamiltonian operator will be written in the form

$$H = H_o + \sum_i H_i \,, \tag{12.1}$$

the operators H_i referring to the separate interactions which make up the total perturbation. The multiplicity of these interactions leads necessarily to a certain complexity of notation. We shall wish to construct complete sets of eigenvectors based at one moment on one subset of the operators H_o, H_i and at another moment on another subset. These various eigen or basis vectors will generally be denoted by symbols of the form $|\alpha_{cijk\ldots}'\rangle$, the indices $0, i, j, k\ldots$ indicating the operators $H_o, H_i, H_j, H_k\ldots$ included in the subset in question. The operator H_o, usually representing the kinetic energy (or simply the remainder after all explicit interactions have been switched off), will be common to all subsets of interest. If scattering is involved it will be necessary to include $\pm$ signs as subscripts in order to distinguish between advanced and retarded wave vectors. When the subset includes <u>all</u> the H_i then the indices will be omitted, and the basis vectors, being then eigenvectors of H, will be written $|\alpha'\rangle$ or $|\alpha_\pm'\rangle$ as usual. Under special circumstances (e.g. for the system described in Figs. 1 to 5 of section 3, which will be analyzed in detail in the present section) the α may be replaced by combinations of the symbols

ζ, J in order to indicate more explicitly the special character--bound, mixed, or free--of the states under consideration.

In each physical situation which comes up for study in the following paragraphs, the central problem involves the construction of the eigenvectors based on one of the subsets from those based on another. As we have seen in all the previous sections such a construction may be expressed formally in terms of the contruction of an operator $\bar{U}(0, -\infty)$ or $\bar{U}(0, \infty)$. We now have to deal with a number of such operators, and to avoid ambiguity we must indicate explicitly which subset is, at any given moment, to be regarded as defining the "unperturbed" eigenvectors and which the "perturbed" eigenvectors. Let the operator sum of one of the subsets be denoted by A and that of the other subset by B. If A is regarded as the "unperturbed" Hamiltonian and B as the "perturbed" Hamiltonian, then the transformation operator in the interaction representation defined by A and B will be denoted by $\bar{U}[B|A](t'', t')$. From Eq. (2.20) we have

$$\bar{U}[B|A](t'', t') = e^{iAt''} e^{-iB(t''-t')} e^{-iAt'} . \qquad (12.2)$$

When a degree of detail is desired which requires A and B to be replaced explicitly by their corresponding sums, a slight abbreviation can be achieved by listing only the pertinent indices on the left side of Eq. (12.2). We shall adopt such a convention. Moreover, in order to conform to previous usage, explicit reference to A and B will be omitted entirely in the case $A = H_0$, $B = H$.

In accordance with these notational developments we shall replace symbols such as $U(t'', t')$, $\bar{U}(0, \mp\infty)$, $R_{\pm}(E)$, $\underset{\sim}{R}_{\pm}$, S, etc., which have been introduced in previous sections for the various basic operators, respectively

by $U[B](t'', t')$, $\bar{U}[B|A](0, \mp\infty)$, $R_{\pm}[B|A](E)$, $\underset{\sim}{R}_{\pm}[B|A]$, $S[B|A]$, etc. In order to avoid excessive clumsiness, however, the operator $\bar{U}[B|A](0, \mp\infty)$, because of its frequent occurrence, will be abbreviated by

$$\bar{U}_{\pm}[B|A] \equiv \bar{U}[B|A](0, \mp\infty) \quad . \tag{12.3}$$

<u>The combination of perturbations.</u>

From Eq. (12.2) one obtains the combination law

$$\bar{U}[C|B](0, t)\,\bar{U}[B|A](0, t) = e^{iCt}\, e^{-iBt}\, e^{iBt}\, e^{-iAt}$$

$$= \bar{U}[C|A](0, t) \quad , \tag{12.4}$$

for finite t. The question immediately arises as to whether this law remains valid when t becomes infinite. More precisely, can one verify the equation

$$\bar{U}_{\pm}[C|B]\,\bar{U}_{\pm}[B|A] = \bar{U}_{\pm}[C|A] \quad , \tag{12.5}$$

the operators being defined by the standard limiting procedure of Eq. (5.22)?

In order to show that Eq. (12.5) <u>is</u> valid we may simply verify that both sides of the equation give the same result when applied to any member of a complete set of eigenvectors of A. We shall begin by considering only free-state eigenvectors of A, which we may denote by $|\zeta_A'\rangle$. Moreover, we shall assume that A, B, C have identical spectra in the continuous range and that the normalization constants involved in the passage from the eigenvectors of one to the eigenvectors of another are all equal to unity. Then, using Eq. (6.1) and remembering that the only role played by ϵ, in the limit $\epsilon \to 0$, is that of determining integration contours, we may write*

* For comments on the analytical theory behind the passage from the first to the second line of Eq. (12.6) see the next section.

$$\bar{U}_{\pm}[C\,|\,A]\,|\zeta_A{}'\rangle = |\zeta_{C\pm}{}'\rangle = \lim_{\epsilon\to 0}\,(E' - C \pm i\epsilon)^{-1}(E' - A \pm i\epsilon)\,|\zeta_A{}'\rangle$$

$$= \lim_{E\to E' \pm i0}\,(E - C)^{-1}\,(E - A)\,|\zeta_A{}'\rangle$$

$$= \lim_{E\to E' \pm i0}\,(E - C)^{-1}(E - B)\,\lim_{E\to E' \pm i0}\,(E - B)^{-1}(E - A)\,|\zeta_A{}'\rangle$$

$$= \lim_{E\to E' \pm i0}\,(E - C)^{-1}(E - B)\,|\zeta_{B\pm}{}'\rangle = \bar{U}_{\pm}[C\,|\,B]\,\bar{U}_{\pm}[B\,|\,A]\,|\zeta_A{}'\rangle, \tag{12.6}$$

where $|\zeta_{B\pm}{}'\rangle$ and $|\zeta_{C\pm}{}'\rangle$ are free-state eigenvectors of B and C respectively, and E' is the corresponding common eigenvalue of A, B and C. Eq. (12.5) is thus proved for the free states.

It is to be noted that Eq. (12.6) may be written in the form

$$|\zeta_{C\pm}{}'\rangle = \bar{U}_{\pm}[C\,|\,B]\,|\zeta_{B\pm}{}'\rangle. \tag{12.7}$$

The important point here is that the $\pm$ signs must go together. This means, for example, that in order to construct the retarded (advanced) wave solutions of a scattering problem one must use "unperturbed" solutions which contain retarded (advanced) waves only, if any.

Eqs. (12.6, 7) may be generalized so as to be valid for bound and mixed states as well as free, and for interacting fields as well as for simpler systems, if level shifts are compensated for by a scheme like that of Eqs. (6.4 - 6) and if appropriate normalization constants are inserted. The resulting generalization of Eq. (12.5) is obviously*

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* It may be noted that Eq. (12.5) actually has perfectly general validity as it stands, although for states in which level shifts are involved it reduces to the triviality $0 = 0$.

$$\bar{\mathcal{U}}_{c\pm}[C|B]\,\bar{\mathcal{U}}_{c\pm}[B|A] = \bar{\mathcal{U}}_{c\pm}[C|A] \,. \tag{12.8}$$

We shall, in the following paragraphs, make frequent use of the generalizations of Eqs. (12.6, 7) for mixed states. However, the simple examples we shall use for illustrative purposes will still be characterized by vanishing level shifts and unit normalization constants (both properties to be verified in each individual case, of course). Therefore we shall simply ignore level shifts and normalization constants, leaving it to the reader to insert them into the mathematical scheme if the nature of the particular application of a formula in which he is interested demands it.

The physical content of Eq. (12.5) (or Eq. (12.8)) is obvious. To obtain the effect of a total perturbation, one may either switch it on all at once or else switch it piecemeal, one part after another * The order of switching, moreover, is immaterial. Similarly, a switch-off process can take place either in a single step or in any number of permutable smaller steps. The complete symmetry between "switch-on" and "switch-off" is emphasized by the equation

$$\bar{U}_{\pm}[C|B] = \bar{U}_{\pm}[B|C]^{*} \,, \tag{12.9}$$

or more generally

$$\bar{\mathcal{U}}_{c\pm}[C|B] = \sum{}' \,|\beta_{C\pm}{}'\rangle\langle\beta_{B\pm}{}'| = \bar{\mathcal{U}}_{c\pm}[B|C]^{*} \,, \tag{12.10}$$

where the $|\beta_{B\pm}{}'\rangle$ are all the eigenvectors of B which have counterparts among the eigenvectors of C, and vice versa.

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* This is <u>strictly</u> true only with respect to states which have counterparts at each step of the switching process.

Scattering by two potentials.

Simple scattering theory provides the most obvious illustration of the utility of the stepwise breakup of the "switch-on" and switch-off" processes. Consider the scattering of a particle by a simple potential which is expressible as the sum of two parts H_1 and H_2 so that

$$H = H_o + H_1 + H_2 \quad . \tag{12.11}$$

Eqs. (12.5) and (12.9) then allow the scattering operator to be written in the form

$$\begin{aligned} S^{\pm 1} &= \bar{U}(\pm\infty, 0)\bar{U}(0, \mp\infty) = \bar{U}_{\mp}[0 \,|\, 0, 1, 2]\, \bar{U}_{\pm}[0, 1, 2 \,|\, 0] \\ &= \bar{U}_{\mp}[0 \,|\, 0, 1]\ \bar{U}_{\mp}[0, 1 \,|\, 0, 1, 2]\ \bar{U}_{\pm}[0, 1, 2 \,|\, 0, 1]\ \bar{U}_{\pm}[0, 1 \,|\, 0] \\ &= \bar{U}_{\mp}[0 \,|\, 0, 1]\, S^{\pm 1}[0, 1, 2 \,|\, 0, 1]\ \bar{U}_{\pm}[0, 1 \,|\, 0] \\ &= \bar{U}_{\mp}[0 \,|\, 0, 1]\left\{ 1 \mp i\, \underset{\sim}{R}_{\pm}[0, 1, 2 \,|\, 0, 1]\right\} \bar{U}_{\pm}[0, 1 \,|\, 0] \\ &= S^{\pm 1}[0, 1 \,|\, 0] \mp i\, \bar{U}_{\mp}[0 \,|\, 0, 1]\, \underset{\sim}{R}_{\pm}[0, 1, 2 \,|\, 0, 1]\ \bar{U}_{\pm}[0, 1 \,|\, 0] \ . \end{aligned} \tag{12.12}$$

Since $S^{\pm 1} = 1 \mp i\, \underset{\sim}{R}_{\pm}$ and $S^{\pm 1}[0, 1 \,|\, 0] = 1 \mp i\, \underset{\sim}{R}_{\pm}[0, 1 \,|\, 0]$, one therefore gets

$$\underset{\sim}{R}_{\pm} = \underset{\sim}{R}_{\pm}[0, 1 \,|\, 0] + \bar{U}_{\mp}[0 \,|\, 0, 1]\, \underset{\sim}{R}_{\pm}[0, 1, 2 \,|\, 0, 1]\, U_{\pm}[0, 1 \,|\, 0] \tag{12.13}$$

Eq. (12.13) finds its chief application when the operator $H_o + H_1$ is sufficiently simple so that its eigenvectors are either exactly or very accurately known. Introducing an obvious notation for the various free-state eigenvectors, and remembering Eqs. (7.1) and (7.45), one may write

Eq. (12.13) in the matrix form

$$\left\langle \zeta_o'' \middle| \underset{\sim}{R}_\pm \middle| \zeta_o' \right\rangle = 2\pi\,\delta(E'' - E')\left[\left\langle \zeta_o'' \middle| H_1 \middle| \zeta_{01\pm}' \right\rangle + \left\langle \zeta_{01\mp}'' \middle| H_2 \middle| \zeta_\pm' \right\rangle\right]$$

$$= 2\pi\,\delta(E'' - E')\left\{\left\langle \zeta_o'' \middle| H_1 \middle| \zeta_{01\pm}' \right\rangle + \left\langle \zeta_{01\mp}'' \middle| H_2 \left[1 - G_{01\pm}(E')H_2\right]^{-1} \middle| \zeta_{01\pm}' \right\rangle\right\}. \tag{12.14}$$

The total scattering amplitude is here displayed as a sum of two parts, one being the <u>known</u> amplitude for scattering by the perturbation H_1 alone, and the other a part which describes the effect of H_2. If H_2 is small Eq. (12.14) immediately suggests an approximation scheme for the total scattering problem based on expansion of the second term inside the curly brackets.

Two important problems, of a type different from that initially envisaged but to which Eq. (12.14) may nevertheless be applied, are the following:

a) <u>Bremsstrahlung.</u> Here H_1 describes the Coulomb field of a nucleus and H_2 the interaction between an electron and the radiation field. The $\left|\zeta_{01\pm}'\right\rangle$ represent Coulomb wave functions. It is important to note that functions of both the retarded and advanced-wave variety are needed in the computation of the second term in (12.14). The vector $\left|\zeta_o'\right\rangle$ describes a state of one electron and no photons, while the vector $\left|\zeta_o''\right\rangle$ denotes a one-electron, one-photon state. The first term in (12.14) evidently makes no contribution to this process. Strictly speaking, Eq. (12.14) must be modified by the usual renormalization procedures if the calculation of the second term is carried out beyond the first order in the binomial expansion.

b) Meson production by nucleon-nucleon collision. This example is quite analogous to the preceding one. Here H_1 may be taken as some sort of phenomenological potential, for which reasonably accurate solutions are known, and H_2 may be chosen as some assumed meson-nucleon coupling.

The example of section 3.

Most of the physical complexities which can occur when several interactions are involved may be illustrated by two-potential examples alone, in particular by the system described in Figs. 1 to 5 of section 3. We therefore turn next to a mathematical description of the possibilities inherent in this system, especially the situations described in Figs. 2, 3 and 4.

Fig. 2 can be disposed of quickly. It represents a simple scattering situation of the standard type, the only new feature being that the unperturbed Hamiltonian is taken as $H_o + H_1$ rather than simply H_o. The transition operator from the state $|\alpha_{01}'\rangle$ to the state $|\alpha_{01}''\rangle$ is given by

$$\begin{aligned}\langle\alpha_{01}''|\underset{\sim}{R}_{\pm}|\alpha_{01}'\rangle &= 2\pi\,\delta(E''-E')\,\langle\alpha_{01}''|H_2|\alpha'\rangle \\ &= 2\pi\,\delta(E''-E')\,\langle\alpha_{01}''|H_2\left[1-G_{01\pm}(E')\,H_2\right]^{-1}|\alpha_{01}'\rangle\end{aligned} \tag{12.15}$$

or, with the more explicit designation of states given in section 3,

$$\begin{aligned}&\langle\zeta_A'', J_{BC}''|\underset{\sim}{R}_{\pm}|\zeta_A', J_{BC}'\rangle \\ &\quad = 2\pi\,\delta(E''-E')\,\langle\zeta_A'', J_{BC}''|H_2\left[1-G_{01\pm}(E')H_2\right]^{-1}|\zeta_A', J_{BC}'\rangle .\end{aligned} \tag{12.16}$$

Here E' and E'' are respectively the sums before and after collision of the kinetic energy of particle A and the internal energy of the bound

system BC. The labels J_{BC}', J_{BC}'' simply describe the internal states of the scatterer.

It is clear that the quantity (12.16) is of order L^{-N} (N being the dimensionality of the space), since its evaluation involves integrations over bound wave functions (independent of L) of particle B and free wave functions (of order $L^{-N/2}$) of particle A multiplied, together with complex conjugates of such functions, by a potential H_2 of (as must be assumed) finite range. In particular, $\mathrm{Im}\,\langle \zeta_A', J_{BC}' | R_\pm | \zeta_A', J_{BC}' \rangle$ has no singular part, and hence the normalization constant Z' is unity.

Disintegrative scattering.

Fig. 3 describes a genuinely new type of process. Here the bound system BC disintegrates as a result of the collision. In order to obtain the transition rate for this process it is convenient to go back to first principles. One is interested in the probability that if, at a certain time t', the system is known to be in a mixed state $|\alpha_{01}'\rangle = |\zeta_A', J_{BC}'\rangle$, it will be found, at a later time t'', in a totally free state $|\alpha_0''\rangle = |\zeta_A'', \bar{J}_{BC}''\rangle$. According to Eq. (1.42) this probability is given by

$$P(\alpha_0'', t'' | \alpha_{01}', t') = \left| \langle \alpha_0'' | U(t'', t') | \alpha_{01}' \rangle \right|^2$$

$$= \left| \langle \alpha_0'' | e^{-iH_0 t''} \bar{U}[0, 1, 2 | 0](t'', 0)\, \bar{U}[0, 1, 2 | 0, 1](0, t') \right.$$
$$\left. e^{i(H_0 + H_1)t'} | \alpha_{01}' \rangle \right|^2$$

$$= \left| \langle \alpha_0'' | \bar{U}[0, 1, 2 | 0](t'', 0)\, \bar{U}[0, 1, 2 | 0, 1] | \alpha_{01}' \rangle \right|^2 . \tag{12.17}$$

In the passage to the second line use is made of Eqs. (2.9) and (12.2).

One can now either form wave packets and then differentiate the transition probability to get the rate, or else one can simply take the limits $t'' \to \pm\infty$, $t' \to \mp\infty$ in Eq. (12.17), via the convention (5.22), and obtain the transition rate formally with the use of the T-symbol. As both methods have been shown in section 8 to lead to the same result, we shall take the easier second alternative. It is to be noted that there is no level shift in the present simple example, so that the limiting convention (5.22) can be applied without difficulty. The normalization constant Z', moreover, is equal to unity as will presently be seen.

Accordingly we write

$$P(\alpha_0'', \pm\infty \,|\, \alpha_{01}', \mp\infty) = \left|\left\langle \alpha_0'' \,\middle|\, \bar{U}_{\mp}[0|0,1,2]\, \bar{U}_{\pm}[0,1,2|0,1] \,\middle|\, \alpha_{01}' \right\rangle\right|^2$$

$$= \left|\left\langle \alpha_0'' \,\middle|\, \bar{U}_{\mp}[0|0,1]\, S^{\pm 1}[0,1,2|0,1] \,\middle|\, \alpha_{01}' \right\rangle\right|^2$$

$$= \left|\left\langle \alpha_{01\mp}'' \,\middle|\, S^{\pm 1}[0,1,2|0,1] \,\middle|\, \alpha_{01}' \right\rangle\right|^2 . \tag{12.18}$$

Here the vector $|\alpha_{01\mp}''\rangle$ denotes a completely free state in which the wave function of particle A is a plane wave but that of particle B has been modified by the scattering effect of the potential H_1. An alternative designation for this state would be $|\zeta_A'', \zeta_{BC\mp}''\rangle$.

Since $\langle \alpha_{01\mp}'' | \alpha_{01}' \rangle = 0$ one obtains immediately the following expression for the transition rate:

$$R(\alpha_0'' | \alpha_{01}') = 2\pi\,\delta(E'' - E')\, \left|\left\langle \alpha_{01-}'' \,\middle|\, R_+[0,1,2|0,1] \,\middle|\, \alpha_{01}' \right\rangle\right|^2$$

$$= 2\pi\,\delta(E'' - E')\, \left|\left\langle \alpha_{01-}'' \,\middle|\, H_2\left[1 - G_{01+}(E')H_2\right]^{-1} \,\middle|\, \alpha_{01}' \right\rangle\right|^2 , \tag{12.19}$$

or

$$R(\zeta_A'', \zeta_B'' | \zeta_A', J_{BC}')$$

$$= 2\pi\,\delta(E'' - E')\left|\left\langle \zeta_A'', \zeta_{BC-}'' \right| H_2\left[1 - G_{01+}(E')H_2\right]^{-1} \left|\zeta_A', J_{BC}'\right\rangle\right|^2 . \tag{12.20}$$

An approximate evaluation of the transition rate based on an expansion of Eq. (12.20) evidently requires an accurate knowledge not only of the bound wave functions of the subsystem BC, but also of its advanced free wave functions.

It is clear that $Z' = 1$, since the pertinent matrix elements are of order $L^{-3N/2}$.

A typical practical example to which Eq. (12.20) or (12.19) may be applied is that of the ejection of a nucleon from a nucleus due to nucleon bombardment. Here both perturbations would be taken as phenomenological potentials, H_1 being that which binds the ejected nucleon to the nucleus and H_2 that which describes the interaction between two individual nucleons.

Two further important applications of Eq. (12.19) (which, however, require the modifications of renormalization theory if calculations are carried out to an order higher than the first) are the following:

a) <u>Deuteron disintegration by pion bombardment.</u> The reaction envisaged is $\pi^+ + d \rightarrow p + p$. Here H_1 is the nucleon-nucleon potential which holds the deuteron together <u>plus</u> the Coulomb repulsion energy which makes its appearance when the neutron becomes a proton through absorption of the π^+. H_2 is the pion-nucleon coupling plus the pion-proton screened Coulomb energy which persists as long as the pion is present.

b) <u>The photoelectric effect.</u> This reaction may be written $\gamma + e_{bound} \rightarrow e_{free}$. Here H_1 is the Coulomb energy which binds the electron in an atom (or in

a metallic lattice) and H_2 is the electron-photon coupling. Very accurate calculations of this process can be made provided that good electronic bound wave functions and advanced free wave functions are known.

Rearrangement collisions.

For the analysis of the process pictured in Fig. 4 we again return to first principles. The transition probability of interest is

$$P(\alpha_{02}'', t'' | \alpha_{01}', t') = \left| \langle \alpha_{02}'' | U(t'', t') | \alpha_{01}' \rangle \right|^2$$

$$= \left| \langle \alpha_{02}'' | e^{-i(H_0 + H_2)t''} \bar{U}[0, 1, 2 | 0, 2](t'', 0) \bar{U}[0, 1, 2 | 0, 1](0, t') e^{i(H_0 + H_1)t'} | \alpha_{01}' \rangle \right|^2$$

$$= \left| \langle \alpha_{02}'' | \bar{U}[0, 1, 2 | 0, 2](t'', 0) \bar{U}[0, 1, 2 | 0, 1](0, t') | \alpha_{01}' \rangle \right|^2 \tag{12.21}$$

where $|\alpha_{01}'\rangle = |\zeta_A', J_{BC}'\rangle$ is the mixed state with particle B bound to C and $|\alpha_{02}''\rangle = |\zeta_T'', J_R''\rangle$ is a mixed state with particles A and B bound together. The over-all probability for the occurrence of this "pick-up" process is given formally by

$$P(\alpha_{02}'', \pm\infty | \alpha_{01}', \mp\infty) = \left| \langle \alpha_{02}'' | \bar{U}_{\mp}[0, 2 | 0, 1, 2] \bar{U}_{\pm}[0, 1, 2 | 0, 1] | \alpha_{01}' \rangle \right|^2$$

$$= \left| \langle \alpha_{\mp}'' | \alpha_{\pm}' \rangle \right|^2 \tag{12.22}$$

where (cf. Eq. (7.6))

$$|\alpha_{\pm}'\rangle = \left[1 + G_{\pm}(E')H_2\right] |\alpha_{01}'\rangle , \tag{12.23}$$

$$|\alpha_{\mp}''\rangle = \left[1 + G_{\mp}(E'')H_1\right] |\alpha_{02}''\rangle . \tag{12.24}$$

For the evaluation of expression (12.22) we need two identities:

$$G_\pm(E'') - G_\pm(E') = -(E'' - E')G_\pm(E'')G_\pm(E') \quad , \tag{12.25}$$

$$\langle \alpha_{02}'' | (H_2 - H_1) | \alpha_{01}' \rangle = (E'' - E') \langle \alpha_{02}'' | \alpha_{01}' \rangle \quad . \tag{12.26}$$

The first follows immediately from Eq. (2.13), and the second becomes obvious if one replaces the difference $H_2 - H_1$ by $(H_o + H_2) - (H_o + H_1)$. Using these identities together with Eqs. (2.15) and (12.23, 24), we may proceed in a manner reminiscent of the derivation of Eq. (7.40).

$$\langle \alpha_\mp'' | \alpha_\pm' \rangle = \langle \alpha_{02}'' | \alpha_{01}' \rangle + \langle \alpha_{02}'' | H_1 \left[1 + G_\pm(E'')H_2 \right] G_{01\pm}(E'') | \alpha_{01}' \rangle$$

$$+ \langle \alpha_{02}'' | G_{02\pm}(E') \left[1 + H_1 G_\pm(E') \right] H_2 | \alpha_{01}' \rangle + \langle \alpha_{02}'' | H_1 G_\pm(E'')G_\pm(E')H_2 | \alpha_{01}' \rangle$$

$$= \langle \alpha_{02}'' | \alpha_{01}' \rangle$$

$$+ \frac{\frac{1}{2}}{E'' - E' \pm i\epsilon} \langle \alpha_{02}'' | \Big\{ H_1 + H_2 - (E'' - E')$$

$$+ H_1 \left[G_\pm(E'') + G_\pm(E') - (E'' - E')G_\pm(E'')G_\pm(E') \right] H_2 \Big\} | \alpha_{01}' \rangle$$

$$+ \frac{\frac{1}{2}}{E' - E'' \pm i\epsilon} \langle \alpha_{02}'' | \Big\{ H_2 + H_1 + (E'' - E')$$

$$+ H_1 \left[G_\pm(E') + G_\pm(E'') + (E'' - E')G_\pm(E'')G_\pm(E') \right] H_2 \Big\} | \alpha_{01}' \rangle$$

$$+ \langle \alpha_{02}'' | H_1 G_\pm(E'')G_\pm(E')H_2 | \alpha_{01}' \rangle$$

$$= \mp i \frac{\epsilon}{(E'' - E')^2 + \epsilon^2} \left\langle \alpha_{02}'' \right| \left\{ H_1 + H_2 + H_1 \left[G_\pm(E'') + G_\pm(E') \right] H_2 \right\} \left| \alpha_{01}' \right\rangle$$

$$+ \frac{\epsilon^2}{(E'' - E')^2 + \epsilon^2} \left\langle \alpha_{02}'' \right| \left[1 + H_1 G_\pm(E'') G_\pm(E') H_2 \right] \left| \alpha_{01}' \right\rangle$$

$$\xrightarrow[\epsilon \to 0]{} \mp 2\pi i \, \delta(E'' - E') \left\langle \alpha_{02}'' \right| \left\{ \tfrac{1}{2}(H_1 + H_2) + H_1 G_\pm(E') H_2 \right.$$

$$\left. \pm \tfrac{1}{2} i\epsilon \left[1 - H_1 \partial G_\pm(E')/\partial E' \, H_2 \right] \right\} \left| \alpha_{01}' \right\rangle . \tag{12.27}$$

The term involving ϵ in the final expression plays a role in renormalization procedures whenever these need to be taken into account. In the present simple example, however, this term may be ignored since the pertinent matrix elements are all of order L^{-N}, there are no "singular parts," and all normalization constants are equal to unity. One therefore gets for the transition rates the three equivalent expressions

$$R(\zeta_T'', J_R'' \,|\, \zeta_A', J_{BC}')$$

$$= 2\pi \delta(E'' - E') \left| \left\langle \zeta_T'', J_R'' \right| \left[\tfrac{1}{2}(H_1 + H_2) + H_1 G_+(E') H_2 \right] \left| \zeta_A', J_{BC}' \right\rangle \right|^2 \tag{12.28a}$$

$$= 2\pi \delta(E'' - E') \left| \left\langle \zeta_T'', J_R'' \right| H_1 \left[1 - G_{01+}(E') H_2 \right]^{-1} \left| \zeta_A', J_{BC}' \right\rangle \right|^2 \tag{12.28b}$$

$$= 2\pi \delta(E'' - E') \left| \left\langle \zeta_T'', J_R'' \right| \left[1 - H_1 G_{02+}(E') \right]^{-1} H_2 \left| \zeta_A', J_{BC}' \right\rangle \right|^2 . \tag{12.28c}$$

The transition rate for the inverse or "stripping" process is evidently obtained from these expressions by interchanging the operators H_1 and H_2

and the labels ζ_A', J_{BC}' and ζ_T'', J_R'', or equivalently by simply changing the + sign attached to the Green's function to a - sign and leaving the expressions as they stand.

Pick-up and stripping processes are collectively termed "rearrangement collisions" since the particles involved suffer a rearrangement in their physical grouping under the collision. The bombardment of nuclei with low energy nuclear particles (light nuclei or individual nucleons) frequently involves rearrangement collisions. These may be of a more complicated type than simple pick-up or stripping processes, involving, for example, a mixture of the two processes. They may, in addition, involve the production of new particles such as photons, electrons, or positrons. Assuming all the pertinent interactions are known, the mathematical theory can be developed along exactly the same lines as for the simple examples above. In practice, however, such a procedure is not of much use owing to the extreme complications of the calculations which then have to be performed. Instead, one generally attempts to deal with simplified models or else rests content with a semi-phenomenological <u>resonance</u> theory of nuclear reactions (see below).

The classic example of the pick-up process is the formation of deuterons when nuclei are bombarded by neutrons. This phenomenon has received much attention in both experiment and theory, as has also the inverse phenomenon, the stripping off of the proton when a deuteron collides with a nucleus. In connection with the stripping process attention should be called to the fact that the stripped particle need not pass over into another bound combination but may instead find itself in a free state after the collision. It is obvious, from the methods of preceding derivations, that the transition rate for this process is given by

$$R(\zeta_A'', \zeta_B'' | \zeta_T', J_R')$$

$$= 2\pi\delta(E'' - E') \left| \left\langle \zeta_A'', \zeta_{BC-}'' \right| H_2 \left[1 - G_{02+}(E')H_1\right]^{-1} \left| \zeta_T', J_R' \right\rangle \right|^2 \tag{12.29a}$$

$$= 2\pi\delta(E'' - E') \left| \left\langle \zeta_A'', \zeta_{BC-}'' \right| \left[1 - H_2 G_{01+}(E')\right]^{-1} H_1 \left| \zeta_T', J_R' \right\rangle \right|^2 . \tag{12.29b}$$

Channels.

The various possible distinct physical groupings in which a given collision may result, or from which collisions may be initiated, are known as channels. The system described in section 3 has three channels as pictured in Figs. 2 to 4. The discussion of the preceding paragraphs has focussed attention on one or another of these channels at a time, but the general similarity of the procedures in each case makes it evident that all the various possible reactions should be describable in terms of one super S-matrix which connects each channel with itself and with all the others. We now proceed to define this matrix.

The procedure is straightforward, except that we must introduce further new notations for the sake of convenience. The states associated with the vectors $\left|\zeta_A', \zeta_B'\right\rangle$, $\left|\zeta_A', J_{BC}'\right\rangle$ and $\left|\zeta_T', J_R'\right\rangle$ will be said to belong to channels number 1, 2 and 3 respectively. The eigenvectors of the total Hamiltonian operator H may be separated into groups corresponding to these channels and will be distinguished by appropriate indices thus:

$$\left|\alpha_{1\pm}'\right\rangle = \bar{U}_{\pm}\left[0, 1, 2 \middle| 0\right] \left|\mathcal{J}_A', \mathcal{J}_B'\right\rangle , \tag{12.30}$$

$$\left|\alpha_{2\pm}'\right\rangle = \bar{U}_{\pm}\left[0, 1, 2 \middle| 0, 1\right] \left|\mathcal{J}_A', J_{BC}'\right\rangle , \tag{12.31}$$

$$\left|\alpha_{3\pm}'\right\rangle = \bar{U}_{\pm}\left[0, 1, 2 \middle| 0, 2\right] \left|\mathcal{J}_T', J_R'\right\rangle . \tag{12.32}$$

It is evident that this scheme separates the eigenvectors of H into three mutually orthogonal sets.* In more complicated examples there may be more than three channesl, but the separation of eigenvectors into orthogonal sets based on the channels is always possible. Thus, in general,

$$P_i P_j = \delta_{ij} P_i , \tag{12.33}$$

where

$$P_i \equiv \sum{}' \left|\alpha_{i\pm}'\right\rangle \left\langle\alpha_{i\pm}'\right| , \qquad i = 1, 2, 3\ldots . \tag{12.34}$$

If the system can have completely bound states $\left|J'\right\rangle$ such as that pictured in Fig. 5 then the $\left|\alpha_{i\pm}'\right\rangle$ do not form a complete set. One must write

$$\sum_i P_i = 1 - P_J \tag{12.35}$$

where

$$P_J \equiv \sum{}' \left|J'\right\rangle \left\langle J'\right| . \tag{12.36}$$

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* The proof that $\left\langle\alpha_{2\pm}''\middle|\alpha_{3\pm}'\right\rangle = 0$ can be carried out explicitly by a derivation similar to that of Eq. (12.27), but using the identity $G_{\mp}(E'') - G_{\pm}(E') = -(E'' - E' \mp 2i\epsilon)G_{\mp}(E'')G_{\pm}(E')$ instead of Eq. (12.25). One obtains a result similar to Eq. (7.11).

Evidently

$$P_i P_J = P_J P_i = 0 \ . \tag{12.37}$$

Now introduce the operators

$$\bar{U}_{1\pm} = \sum{}' \left|\alpha_{1\pm}'\right\rangle \left\langle \zeta_A', \zeta_B' \right| , \tag{12.38}$$

$$\bar{U}_{2\pm} = \sum{}' \left|\alpha_{2\pm}'\right\rangle \left\langle \zeta_A', J_{BC}' \right| , \tag{12.39}$$

$$\bar{U}_{3\pm} = \sum{}' \left|\alpha_{3\pm}'\right\rangle \left\langle \zeta_T', J_R' \right| , \tag{12.40}$$

or similar operators for more complicated systems. The super S-matrix for the system is then defined by

$$S^{\pm 1} = \left(S^{\pm 1}{}_{ij} \right) , \tag{12.41}$$

$$S^{\pm 1}{}_{ij} = \bar{U}_{i\mp}{}^{*} U_{j\pm} = S^{\mp 1}{}_{ji}{}^{*} \ . \tag{12.42}$$

The various transition rates which have been calculated in previous paragraphs are directly proportional to the squares of the absolute values of appropriate elements of this matrix.

The unitarity of the super S-matrix is readily demonstrated. We note the identities

$$P_J \bar{U}_{i\pm} = 0 \ , \tag{12.43}$$

$$\bar{U}_{i\pm} \bar{U}_{i\pm}{}^{*} = P_i \ , \tag{12.44}$$

and then, using Eq. (12.35), write (cf. Eq. (7.32))

$$\sum_k S^{\pm 1}_{ki}{}^* S^{\pm 1}_{kj} = \sum_k S^{\mp 1}_{ik} S^{\mp 1}_{jk}{}^*$$

$$= \sum_k \bar{U}_{i\pm}{}^* \bar{U}_{k\mp} \bar{U}_{k\mp}{}^* \bar{U}_{j\pm} = \bar{U}_{i\pm}{}^* (1 - P_J) \bar{U}_{j\pm}$$

$$= \bar{U}_{i\pm}{}^* \bar{U}_{j\pm} = \underset{\sim}{1}_{ij} , \tag{12.45}$$

where

$$\underset{\sim}{1}_{ij} = 0 , \qquad i \neq j , \tag{12.46}$$

$$\underset{\sim}{1}_{11} = \sum{}' \left| \zeta_A{}', \zeta_B{}' \right\rangle \left\langle \zeta_A{}', \zeta_B{}' \right| , \tag{12.47}$$

$$\underset{\sim}{1}_{22} = \sum{}' \left| \zeta_A{}', J_{BC}{}' \right\rangle \left\langle \zeta_A{}', J_{BC}{}' \right| , \tag{12.48}$$

$$\underset{\sim}{1}_{33} = \sum{}' \left| \zeta_T{}', J_R{}' \right\rangle \left\langle \zeta_T{}', J_R{}' \right| , \tag{12.49}$$

with appropriate generalizations for more complicated systems.

Resonances.

When the number of channels is large, or if the system is rather complex, or if the various interactions are not all known explicitly, then it is not feasible to compute the super S-matrix directly. Instead, a theory based on the existence (observed or assumed) of metastable, or excited, states is often useful. A theory of this type, known as the Wigner-Eisenbud theory [134 to 139], is one of the principal tools used in the analysis of nuclear reactions. The motivation behind it is simple.

The phenomenon of excitation and subsequent decay is frequently observed in nuclear reactions, together with all that this implies in regard to level structure, level widths and lifetimes. It is natural to picture

the physical process involved as one in which the initiators of a reaction (i.e. the individual particle groups which initially collide with one another) come together to form a single compound nucleus. Since energy is conserved in a collision the arguments given in sections 3 and 11 imply that the compound nucleus can only be formed in an excited state which must then proceed to decay. If the decay rate is slow enough the decay process may be directly observed. Many of the level widths, however, may be large enough so that the decay process is completely unobservable. The existence of the corresponding excited levels can nevertheless make itself known through resonances in the cross sections for various nuclear reactions.

The method of approach to a mathematical description of nuclear resonance phenomena is obvious. One places around the compound nucleus a fictitious potential barrier, the removal of which is regarded as an additional perturbation. The general form of the transition matrix for the various possible processes may be inferred from the simple example considered in section 11, namely

$$R_{\pm ba} \approx \sum_{\gamma} \frac{X_{b\gamma} X_{a\gamma}^{*}}{E_a - E_\gamma \pm \frac{1}{2} i \Gamma_\gamma} , \tag{12.50}$$

where

$$\Gamma_\gamma = 2\pi \sum_a \delta(E_a - E_\gamma) \left| X_{a\gamma} \right|^2 . \tag{12.51}$$

Here the labels a, b refer to states in various channels, and the index refers to the excited levels of the compound nucleus. The $X_{a\gamma}$ are parameters which give a measure of the extent to which the compound nuclear wave function overlaps the various channel wave functions in the region occupied by the

potential barrier. If the level widths Γ_γ are small compared to the level separations then the $X_{a\gamma}$ may be chosen as energy independent, and

$$2\pi \sum_b \delta(E_b - E_a) \left| R_{\pm ba} \right|^2$$

$$\approx 2\pi \sum_{b,\gamma} \delta(E_b - E_\gamma) \frac{\left|X_{b\gamma}\right|^2 \left|X_{a\gamma}\right|^2}{(E_a - E_\gamma)^2 + \frac{1}{4}\Gamma_\gamma^2}$$

$$= \sum_\gamma \Gamma_\gamma \frac{\left|X_{a\gamma}\right|^2}{(E_a - E_\gamma)^2 + \frac{1}{4}\Gamma_\gamma^2} \approx \mp 2 \operatorname{Im} R_{\pm aa} , \tag{12.52}$$

so that conservation of probability (at least approximately) is automatic.*

In order that Eq. (12.50) be really useful the potential barrier must, as we have seen in the preceding section, be chosen carefully so that the normalization constants $Z_{\pm\gamma}$ for the excited levels are nearly equal to unity. In standard presentations of the theory [134, 137] the potential barrier is usually never mentioned as such, being replaced simply by a hypersurface in coordinate space, with respect to which one can define a convenient set of orthonormal compound nuclear wave functions satisfying definite boundary conditions. The careful placing of this surface, which is necessary for numerical estimates of the various physical parameters, is quite equivalent to the careful choice of potential barrier.

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* Conservation of probability and unitarity of the super S-matrix follow rigorously if one works with the reactance matrix instead of dealing directly with the transition matrix. The reactance matrix is (apart from certain simple factors) just the "derivative matrix" of Wigner and Eisenbud, and has the form

$$K_{ba} = \sum_\gamma \frac{X_{b\gamma} X_{a\gamma}^*}{E_a - E_\gamma} .$$

In given instances the values of some of the parameters $X_{a\gamma}$ can actually be estimated on the basis of knowledge of nuclear structure. It would carry us too far afield, however, to go into the details of such calculations. Even when the $X_{a\gamma}$ cannot be computed Eq. (12.50) is quite useful in the correlation of theory with experiment. If obvious factors involving densities of states are correctly accounted for, values for these parameters may be inferred from the observed behavior with energy of the various cross sections. It turns out that Eq. (12.50) has a wide range of validity, even when the level widths cannot be strictly regarded as small.

Multiple scattering.

Although for the problems just considered the multiplicity of various interactions makes a direct approach out of the question, there is a class of problems involving large numbers of interactions H_i in which exact expressions for the transition amplitudes are useful. These are the problems in which a single particle is scattered by several different centers of force. The simplifying features of such problems which make the exact expressions useful are generally either that the scattering centers are arranged in a regular array (e.g. a crystal lattice) or else that the scatterers satisfy special statistics (indistinguishability). Sometimes the exact expression is desired not to make use of it in an actual calculation but simply to obtain an estimate of the error involved in replacing it by an approximation (e.g., the error involved in ignoring nuclear opacity in the calculation of the scattering of particles by nuclei).

The exact transition operator is the solution of the integral equation

$$R_{\pm}(E) = \sum_i H_i \left[1 + G_{o\pm}(E) R_{\pm}(E) \right] \qquad (12.53)$$

Here the H_i represent the interactions between the scattered particle and the various scatterers. If the scatterers are held fixed the unperturbed Hamiltonian H_o is simply the kinetic energy of the scattered particle, but if the scatterers are not completely rigid H_o must include their kinetic energies plus the potential which binds them.

What is desired is to reexpress $R_\pm(E)$ in terms of the transition operators

$$R_{i\pm}(E) = H_i \left[1 + G_{o\pm}(E)\, R_{i\pm}(E) \right] \tag{12.54}$$

which describe the scattering produced by each individual scatterer [140, 141, 143]. For this purpose it is convenient to introduce operators $\Omega_{i\pm}(E)$ satisfying the following set of coupled integral equations:

$$\Omega_{i\pm}(E) = 1 + G_{o\pm}(E) \sum_{j \neq i}{}_j\, R_{j\pm}(E)\Omega_{j\pm}(E) , \qquad i = 1, 2, 3 \ldots \tag{12.55}$$

The total transition operator may then be expressed in the form

$$R(E) = \sum_i H_i \left[1 + G_{o\pm}(E) \sum_j R_{j\pm}(E)\Omega_{j\pm}(E) \right] , \tag{12.56}$$

as may be verified by showing that the expression on the right satisfies the integral equation (12.53). Thus

$$\begin{aligned}
&\sum_i H_i \left\{ 1 + G_{o\pm}(E) \sum_j H_j \left[1 + G_{o\pm}(E) \sum_k R_{k\pm}(E)\Omega_{k\pm}(E) \right] \right\} \\
&= \sum_i H_i \left\{ 1 + G_{o\pm}(E) \sum_j H_j \left[1 + G_{o\pm}(E) \sum_{k \neq j}{}_k R_{k\pm}(E)\Omega_{k\pm}(E) \right.\right. \\
&\qquad \left.\left. + G_{o\pm}(E) R_{j\pm}(E)\Omega_{j\pm}(E) \right] \right\} \\
&= \sum_i H_i \left\{ 1 + G_{o\pm}(E) \sum_j H_j \left[1 + G_{o\pm} R_{j\pm}(E) \right] \Omega_{j\pm}(E) \right\} \\
&= \sum_i H_i \left[1 + G_{o\pm}(E) \sum_j R_{j\pm}(E)\Omega_{j\pm}(E) \right] .
\end{aligned} \tag{12.57}$$

A more useful form of expression (12.56) may be obtained by splitting off the ith term in the second sum and making use of Eqs. (12.54, 55). One easily finds [143]

$$R_{\pm}(E) = \sum_i R_{i\pm}(E)\left[1 + G_{o\pm}(E) \sum_{j\neq i}{}_j R_{j\pm}(E)\Omega_{j\pm}(E)\right]$$

$$= \sum_i R_{i\pm}(E) + \sum_i R_{i\pm}(E)G_{o\pm}(E) \sum_{j\neq i}{}_j R_{j\pm}(E)$$

$$+ \sum_i R_{i\pm}(E)G_{o\pm}(E) \sum_{j\neq i}{}_j R_{j\pm}(E)G_{o\pm}(E) \sum_{k\neq j}{}_k R_{k\pm}(E) + \cdots \quad . \tag{12.58}$$

Eq. (12.58) corresponds to a physical description of the total scattering process as the sum of all possible single scatterings, double scatterings, triple scatterings, etc. It is, of course, the amplitudes rather than the individual probabilities which must be summed to give the total scattering. If the scatterers are sufficiently few and far apart, the operator $R_{\pm}(E)$ may be approximated by

$$R_{\pm}(E) \approx \sum_i R_{i\pm}(E) \quad . \tag{12.59}$$

<u>Some comments.</u>

It is in problems involving several perturbations that the greatest potentialities exist for the introduction of formal tricks leading to a reduction in the labor involved in obtaining numerical answers. These tricks usually take the forms of justifications for various simplifying approximations and may range all the way from scrupulously honest and accurate estimates of errors involved to arguments of the conscience-salving variety. As indicated in the Introduction we shall not devote space in this article to descriptions of these tricks. However, the reader will by

now have at his command all the formal apparatus he needs to read the pertinent literature with ease. We shall simply call attention to two outstanding examples which illustrate the utility of the formal theory: 1) the justification of the so-called impulse approximation [147 to 152] and 2) the justification of the so-called optical model for nuclei [143].

The impulse approximation applies to the scattering of a free particle by a bound particle under circumstances for which it is not useful to employ Eqs. (12.15, 16), namely, when the binding potential H_1 rather than the scattering potential H_2 may be regarded as weak and when the eigenvectors of the operator $H_0 + H_2$ rather than of $H_0 + H_1$ are known (or can be inferred from the results of scattering experiments between free particles). The statement of the impulse approximation is essentially that the scattering due to the bound particle can be computed from the free-particle scattering amplitudes simply by summing over the momentum distribution of the bound particle. Applied in reverse, in combination with experiment, the impulse approximation provides a tool for the direct measurement of nuclear wave functions and hence of the nuclear potential.

The justification of the optical model has been carried out by Francis and Watson. It is an argument which permits Eq. (12.53) to be replaced for a nucleus by an approximate equation

$$R_{\pm}(E) \approx \mathcal{V}(E)\left[1 + \mathcal{G}_{o\pm}(E)R_{\pm}(E)\right] , \qquad (12.60)$$

where $\mathcal{G}_{o\pm}(E)$ is the Green's function for the scattered particle alone and $\mathcal{V}(E)$ is an energy dependent operator which is diagonal in the coordinate representation of the scattered particle and which corresponds to a fictitious potential, constant inside the nucleus and vanishing outside. $\mathcal{V}(E)$ is known as the "optical potential;" its dependence on energy means

that it is not a potential of the ordinary type. Its approximate existence depends critically on the fact that the scatterers (i.e. the particles composing the nucleus) satisfy Fermi statistics. Absorption effects may be taken into account by giving $\mathcal{V}(E)$ an imaginary part.

Attention may also be called to some work of Brueckner [145, 146] which has certain formal similarities with that of Francis and Watson. Brueckner's problem is that of determining nuclear binding energies from nucleon-nucleon scattering data. The circumstances of his problem permit the establishment of a remarkable connection between bound-state or discrete-level theory and continuum theory.* Again the Fermi statistics of the nuclear particles are crucial.

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* Unfortunately the rigorous derivation of this connection is not properly carried out by Brueckner. See, however, A. Reifman, B. S. DeWitt, and R. G. Newton, Phys. Rev. (to be published).

13. FINAL REMARKS

We have now reached a logical stopping place. To carry the development of perturbation theory further would require less attention to be paid to the purely formal aspects of the theory and more to the individual mathematical details of particular systems or particular physical situations. Already we have particularized to a considerable extent in the section on field theories. But this was necessary in order to illustrate the full range of mathematical possibilities inherent in the seemingly innocent symbols H, H_o, $R_\pm$, etc. with which one plays in the operator formalism. To particularize any further would change the point of view of the article, even if questions of space were irrelevant.

There remain, nevertheless, several broad fields of investigation within perturbation theory which can be, and have been, developed with a minimum of particularization and into which one can easily pass from the operator formalism itself. It is appropriate to call attention in closing to a number of these "theories within theories" which are of considerable current interest:

1) Variational formulations. We place this topic first because of its great practical importance. The lack of a discussion of variational methods as applied to quantum perturbation theory constitutes perhaps the most serious omission of the present article, especially since most of the theory is quite general and independent of the physical details of the systems H and H_o. Moreover, a coherent presentation of techniques and a comprehensive collection of formulae is definitely wanted in the literature. The author can only plead lack of time and space and refer the reader to the list of references [155 to 185] in the bibliography at the end of the article.

The chapter on variational methods in reference [10] provides probably the best introduction to the subject as far as modern applications go.

2) Time reversal. Much less serious is the omission from this article of any discussion of the extra relations that can be derived between basic operators such as R_+ and R_- when the condition of invariance under time reversal is imposed on the operators H and H_0. A very complete account of the whole subject can be found in the article by Watanabe [154], and a good statement-in-a-nutshell of the application to scattering can be found in an appendix by Chew and Goldberger [150].

3) Construction of a potential from the Phase shift [186 - 192]. The most general statement of this problem is: Given H_0 and the S-matrix, find the perturbation H_1. Its interest obviously lies in the fact that scattering experiments often provide the only means we have of determining the nature of interactions between elementary particles. It is evident, however, that the solution of this problem is highly underdetermined. A knowledge of the S-matrix gives information only about the asymptotic behavior of wave functions. Their behavior in the scattering region must also be known in order to determine the exact form of the perturbation. Stated in another way, H_1 has many more nonvanishing matrix elements than S. (The nonvanishing matrix elements of S all lie on the energy shell.) Hence the number of unknowns far exceeds the number of given quantities.

It is therefore remarkable that H_1 may still be completely determined by S, or at least reduced to a member of a finite-parameter family, if one makes the additional assumption that H_1 is diagonal in some particular complete set of variables. The diagonalizing variables are usually taken to be the configuration coordinates of the system, and only

part of the S-matrix is assumed known, e.g., in three dimensions, the s-phase shift at all energies for scattering by an assumed spherically symmetric potential. If the phase shifts are also known for other angular momenta then H_1 may actually be overdetermined; i.e., the form of the S-matrix may be incompatible with the assumed identification of the variables which diagonalize H_1.

There is also some evidence* that the knowledge of the phase shifts at a single energy only, but for all angular momenta, is sufficient to determine H_1, again provided H_1 is assumed diagonal in the coordinates.

The assumption of a particular set of diagonalizing variables is, of course, a principal drawback of these investigations as far as practical applications are concerned. In thus drastically reducing the generality of the context of the theory the assumption also forces an inescapable specialization in the mathematics used. Details, for example, concerning integrability and boundary conditions on simple central-force potentials become of importance. These investigations have, however, revealed information of a general interest on the role played by bound states in scattering theory. Also the use made of complex function theory shows that much additional information about the consequences of general perturbation theory may be gained by introducing the methods of mathematical analysis in new ways.

4) Causality and dispersion relations [193 to 210].

One of the most fruitful applications of mathematical analysis, in affording insight into the actual content of a given theory, has been the study of the behavior of operators such as $R_{\pm}(E)$ and $G_{\pm}(E)$ or of functions such as $\langle E', \lambda' | S | E', \lambda' \rangle$ and $\langle E', \lambda' | \underset{\sim}{K} | E', \lambda' \rangle$ in the complex energy plane. Some use of the complex E-plane has already been made in this article, in the contour

* Private communication from Professor J. A. Wheeler.

integrations of section 9 and in the characterization of excited states in section 11. In fact, the operator formalism could have been generalized at the outset to include the whole complex plane, the perturbed state-vectors $|\alpha_{\pm}'\rangle$ being definable as follows:

$$Z'^{\frac{1}{2}} |\alpha_{\pm}'\rangle = \lim_{E \to E' \pm i0} |\alpha', E\rangle , \tag{13.1}$$

where

$$\begin{aligned} |\alpha', E\rangle &= (E - H)^{-1} (E - H_o) |\alpha_o'\rangle \\ &= \left[1 - G_o(E) H_1\right]^{-1} |\alpha_o'\rangle \\ &= \left[1 + G_o(E)\, R(E)\right] |\alpha_o'\rangle , \end{aligned} \tag{13.2}$$

$$G_o(E) = (E - H_o)^{-1} , \tag{13.3}$$

$$R(E) = H_1 \left[1 + G_o(E)\, R(E)\right] . \tag{13.4}$$

This possibility has already been pointed out in connection with the derivation of Eq. (12.6) of the preceding section. The advantages of this approach lie in an improved treatment of the limiting process involved in Eq. (6.8) and also in a more comprehensive analysis of the solutions of the integral equation (13.4). The kernel $H_1\, G_o(E)$ of the latter equation depends on two parameters, E and the coupling constant g. By considering both parameters in the complex plane important relations between energy levels, phase shifts, and coupling constant may be inferred.

Much work has been done in applying complex function theory to the study of the consequences of certain very simple and plausible assumptions about the nature of the interaction H_1 in various special systems. These assumptions take the form of statements that the interaction satisfies

certain principles of causality which may be rigorously defined, and which have to do with such things as the finite size of the scattering region and the impossibility of producing a scattering effect before an initial signal (or wave packet) has reached the scatterer. In given instances these assumptions allow the inferrence of certain properties of the behavior of various operators and matrix elements (particularly the S-matrix) in the complex energy plane. These properties in turn permit the invocation of standard theorems of complex function theory which establish relations between such things as the real and imaginary parts of forward scattering amplitudes, or which yield explicit canonical forms for the S-matrix.

Although their results are limited in each case to the specific system H_o under consideration, investigations into the consequences of causality have a surprising range of applicability. For example, the general form (12.50) of the transition operator for nuclear systems may be inferred on causal grounds alone (plus the assumption of a finite boundary for the compound nucleus) [197 to 203]. On the other hand, to take an example from field theory, recent researches [207 to 210] have shown that expression (10.124) for the transition operator for meson scattering has an essentially causal structure. These and many other illustrations of the implications of causality conditions may be found in the references in the bibliography.

5) Fredholm theory. Mention of the Fredholm theory has been made only briefly in this article--in section 9 on bound-state theory. The omission of any reference to the Fredholm theory in connection with scattering has been due to the unfortunate fact that it has not had a very great practical utility for free-state problems--certainly not as great as one might have expected in view of the strong statements about convergence which can be made within

its context. For the sake of completeness, however, we shall here very briefly indicate, in quantum mechanical dress, the starting point of the Fredholm theory.

One forms (formally) the determinant

$$D(E) = \det\left[1 - G_o(E)\, H_1\right] , \tag{13.5}$$

and then, making an infinitesimal variation in the perturbation H_1 and using the formal identity $(\det A)^{-1}\, \delta\, (\det A) = \mathrm{Tr}\, A^{-1}\, \delta A$ for an arbitrary operator (matrix) A, one writes

$$\delta D(E) = -D(E)\, \mathrm{Tr}\, G(E)\, \delta H_1 \tag{13.6}$$

where

$$G(E) = (E - H)^{-1} = \left[1 - G_o(E)\, H_1\right]^{-1} G_o(E) . \tag{13.7}$$

Eq. (13.6) allows the Green's function $G(E)$ to be expressed as a variational derivative:

$$G(E) = -\left[\delta D(E)/\delta H_1\right]/D(E) = -\delta \ln D(E)/\delta H_1 . \tag{13.8}$$

When continuum eigenvalues are involved it is, of course, not immediately clear how to form the determinant $D(E)$. The problem can, however, be entirely transformed into the problem of evaluating traces by noting that Eq. (13.6) may be formally integrated to give

$$\ln D(E) = \mathrm{Tr}\, \ln\left[1 - G_o(E)\, H_1\right] , \tag{13.9}$$

and hence

$$\det\left[1 - G_o(E)\, H_1\right] = \exp \mathrm{Tr}\, \ln\left[1 - G_o(E)\, H_1\right] . \tag{13.10}$$

In one-dimensional problems $D(E)$ (and hence also its variational derivative) is generally an entire function of the coupling constant g. Eq. (13.8) therefore expresses the Green's function as the ratio of two entire functions. For problems of more than one dimension, however, $D(E)$ generally diverges and must be replaced by

$$D^{(1)}(E) = D(E) \exp \mathrm{Tr}\, G_o(E)\, H_1$$
$$= \exp \mathrm{Tr} \left\{ \ln \left[1 - G_o(E)\, H_1 \right] + G_o(E)\, H_1 \right\} , \tag{13.11}$$

in terms of which one may write

$$G(E) = G_o(E) - \delta \ln D^{(1)}(E)/\delta H_1 . \tag{13.12}$$

$D^{(1)}(E)$ is often an entire function of g even when $D(E)$ is not.

Applications of the Fredholm theory to field theories may be found in references [211] to [216].

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BIBLIOGRAPHY

General reference books.

Perturbation theory of a classical field:

[1] J. W. S. Rayleigh, Theory of Sound, MacMillan, London (1896).

Old quantum theory:

[2] M. Born, The Mecanics of the Atom, G. Bell and Sons, London (1927).

Modern quantum theory:

[3] E. C. Kemble, The Fundamental Principles of Quantum Mechanics, McGraw-Hill, New York (1937).

[4] P. A. M. Dirac, The Principles of Quantum Mechanics, Third edition, Oxford (1947).

[5] N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions, Oxford (1948).

[6] W. Pauli, Meson Theory of Nuclear Forces, Second edition, Interscience Publishers, New York (1948).

[7] G. Wentzel, Quantum Theory of Fields, Interscience Publishers, New York (1949).

[8] W. Heitler, The Quantum Theory of Radiation, Third edition, Oxford (1954).

[9] J. M. Blatt and V. F. Weisskopf, Theoretical Nuclear Physics, John Wiley and Sons, New York (1952).

[10] P. M. Morse and H. Feshbach, Methods of Theoretical Physics, McGraw-Hill, New York (1953).

Transformation operators and the time ordering device.

[11] F. J. Dyson, Phys. Rev. 75, 486 (1949).

[12] R. P. Feynman, Phys. Rev. 84, 108 (1951).

[13] I. Fujiwara, Prog. Theor. Phys. 7, 433 (1952).

Retarded and advanced waves.

[14] P. A. M. Dirac, Proc. Roy. Soc. (London), A167, 148 (1938).

Scattering theory (general).

[15] J. Schwinger, unpublished Harvard lectures (various years).

[16] F. E. Low, Seminar on scattering theory, hectographed notes, University of Illinois (1953).

See also the general reference books, in particular [5], for a complete discussion of most aspects of scattering theory.

The S-matrix.

[17] J. A. Wheeler, Phys. Rev. 52, 1107 (1937).

[18] E. C. G. Stueckelberg, Helv. Phys. Acta 17, 13 (1943).

[19] W. Heisenberg, Z. Physik 120, 513, 673 (1943).

[20] C. Møller, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. 23, No. 1 (1945); 22, No. 19 (1946).

Structure of the S-matrix.

[21] K. Wildermuth, Z. Physik 127, 85 (1949).

[22] E. C. G. Stueckelberg and D. Rivier, Helv. Phys. Acta 23, 215 (1950).

[23] N. G. van Kampen, Phil. Mag. 42, 851 (1951).

[24] R. J. Eden, Proc. Roy. Soc. (London) A199, 256 (1949); A215, 133 (1952); A217, 390 (1953); A219, 109, 516 (1953).

[25] M. Moshinsky, Phys. Rev. 91, 984 (1953).

[26] Y. Nambu, Phys. Rev. 98, 803 (1955).

See also references [134] to [139] and [193] to [210].

Formal theory of scattering (general).

[27] E. Feenberg, Phys. Rev. 74, 664 (1948).

[28] M. L. Goldberger, Phys. Rev. 82, 757 (1951); 84, 1008 (1951).

[29] M. Schönberg, Nuovo cimento 8, 651 (1951).

[30] M. Gell-Mann and M. L. Goldberger, Phys. Rev. 91, 398 (1953)

[31] S. T. Epstein, Phys. Rev. 98, 196 (1955).

[32] B. S. DeWitt, Phys. Rev. 100

See Also references [33] and [160].

Limiting procedures, adiabatic switching, level shifts, etc.

[33] M. Schönberg, Nuovo cimento 8, 243, 403 (1951).

[34] M. Gell-Mann and F. E. Low, Phys. Rev. 84, 350 (1951), (Appendix).

[35] B. Ferretti, Nuovo cimento 8, 108 (1951).

[36] H. S. Snyder, Phys. Rev. 83, 1154 (1951).

[37] S. Fubini, Nuovo cimento 9, 846 (1952).

[38] ---, Atti. Accad. Naz. Lincei 12, 298 (1952).

[39] S. T. Ma, Phys. Rev. 87, 652 (1952); 88, 1211 (1952).

[40] H. Suura, Y. Mimura, and T. Kimura, Prog. Theor. Phys. 7, 171 (1952).

[41] ---, Prog. Theor. Phys. 12, 49 (1954), (esp. appendices).

[42] F. J. Belinfante and C. Møller, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd., 28, No. 6 (1953).

[43] M. N. Hack, Phys. Rev. 96, 196 (1954).

[44] F. Coester, M. Hamermesh, and K. Tanaka, Phys. Rev. 96, 1142 (1954).

[45] H. E. Moses, Nuovo cimento 1, 103 (1955).

Convergence in simple scattering theory.

[46] R. Jost and A. Pais, Phys. Rev. 82, 840 (1951).

[47] R. H. Dalitz, Proc. Roy. Soc. (London) A206, 509 (1951).

[48] S. T. Ma, Phys. Rev. 91, 392 (1953).

[49] W. Kohn, Revs. Modern Phys. 26, 292 (1954).

Bound state perturbation theory.

Old quantum theory:

[50] M. Born, reference [2] , chapter 4.

Modern quantum theory:

[51] M. Born, W. Heisenberg, and P. Jordan, Z. Physik 35, 557 (1925).

[52] E. Schrödinger, Ann. Physik 80, 437 (1926).

[53] E. Feenberg, Phys. Rev. 74, 206 (1948).

[54] P. I. Richards, Phys. Rev. 74, 835 (1948).

[55] H. Feshbach, Phys. Rev. 74, 1548 (1948).

[56] T. Kato, Prog. Theor. Phys. 4, 514 (1949); 5, 95, 207 (1950).

[57] ---, Phys. Rev. 77, 413 (1950).

[58] E. A. Power, Proc. Roy. Soc. (London) A218, 384 (1953).

[49] A. Cunliffe and R. N. Gould, Phil. Mag. 44, 785 (1953); 45, 818 (1954).

See also references [3], [4], [10], and [33].

The adiabatic theorem.

Old quantum theory:

[60] M. v. Laue, Ann. Physik 76, 619 (1925).

[61] P. A. M. Dirac, Proc. Roy. Soc. (London) A107, 725 (1925).

[62] M. Born, reference [2], chapter 2, § 10, p.52, § 16, p.95.

Modern quantum theory:

[63] M. Born and V. Fock, Z. Physik 51, 165 (1928).

See also references [33] and [45].

Convergence in bound state perturbation theory.

[64] F. Rellich, Math. Ann. 113, 600, 677 (1937); 116, 555 (1939); 117, 356 (1940).

See also reference [56].

Heitler integral equation, radiation damping, and reactance operator.

[65] I. Waller, Z. Physik 88, 436 (1934).

[66] W. Heitler, Proc. Cambridge Phil. Soc. 37, 291 (1941).

[67] --- and H. W. Peng, Proc. Cambridge Phil. Soc. 38, 296 (1942).

[68] --- and S. T. Ma, Phil. Mag. 40, 651 (1949).

[69] ---, reference [8], §§ 15 and 16.

[70] A. H. Wilson, Proc. Cambridge Phil. Soc. 37, 301 (1941).

[71] A. Sokolov, J. Phys. U.S.S.R. 5, 231 (1941).

[72] E. Gora, Z. Physik 120, 121 (1943).

[73] S. T. Ma and C. F. Hsueh, Proc. Cambridge Phil. Soc. 40, 167 (1944).

[74] J. Pirenne, Helv. Phys. Acta 21, 226 (1948).

[75] ---, Phys. Rev. 86, 395 (1952).

[76] W. Pauli, reference [6], chapter IV.

[77] N. Fukuda and T. Miyazima, Prog. Theor. Phys. 5, 849 (1950).

[78] J. Hamilton, Proc. Phys. Soc. (London) 62A, 2, 12, 749, 1036 (1950).

[79] M. Schönberg, Nuovo cimento 8, 651 (1951).

[80] S. N. Biswas, Phys. Rev. 91, 1026 (1953); 94, 1767 (1954).

See also reference [33].

Decay, line shape, and resonance scattering.

[81] V. F. Weisskopf and E. P. Wigner, Z. Physik 63, 54 (1930); 65, 18 (1932).

[82] K. O. Friedrichs, Comm. Appl. Math. 1, 361 (1948).

[83] W. Heitler and S. T. Ma, Proc. Roy. Ir. Acad. 52, 109 (1949).

[84] E. C. Titchmarsh, Proc. Roy. Soc. (London) A200, 34 (1949); A201, 473 (1950); A207, 321 (1951); A210, 30 (1951).

[85] M. Schönberg, Nuovo cimento 8, 817 (1951).

[86] E. Arnous and S. Zienau, Helv. Phys. Acta 24, 279 (1951).

[87] --- and K. Bleuler, Helv. Phys. Acta 25, 581 (1952).

[88] ---, Helv. Phys. Acta 25, 631 (1952).

[89] --- and W. Heitler, Proc. Roy. Soc. (London) A220, 290 (1953).

[90] F. E. Low, Phys. Rev. 88, 53 (1952).

[91] E. J. Hellund, Phys. Rev. 89, 919 (1953).

See also reference [24].

Renormalization of simple field theories.

[92] G. F. Chew, Phys. Rev. 94, 1748, 1755 (1954); 95, 285 (1954).

[93] F. E. Low, Proceedings of the Fifth Annual Rochester Conference on High Energy Nuclear Physics, University of Rochester (1955).

[94] G. F. Chew and F. E. Low. 1) Theory of p-wave pion nucleon interaction at low energies. 2) Theory of photo-meson production at low energies. (To be published.)

Threshold theorems.

[95] W. Thirring, Phil. Mag. 41, 1193 (1950).

[96] N. M. Kroll and M. A. Ruderman, Phys. Rev. 93, 233 (1954).

[97] S. Deser, M. L. Goldberger, and W. Thirring, Phys. Rev. 94, 711 (1954).

[98] F. E. Low, Phys. Rev. 96, 1428 (1954).

[99] ---, Phys. Rev. 97, 1392 (1955).

[100] M. Gell-Mann and M. L. Goldberger, Phys. Rev. 96, 1433 (1954).

[101] S. Fubini, Nuovo cimento 2, 180 (1955).

[102] M. Cini and S. Fubini, Nuovo cimento 2, 192 (1955).

[103] A. Klein, Low energy theorems for renormalizable field theories. (To be published.)

Structure of propagation functions.

[104] H. Lehmann, Nuovo cimento 11, 342 (1954).

[105] J. G. Valatin, Proc. Roy. Soc. (London) A225, 535 (1954).

[106] P. T. Matthews and A. Salam, Nuovo cimento 2, 120 (1955).

[107] S. F. Edwards, Proc. Roy. Soc. (London) A228, 411 (1955).

Solvable field theories.

[108] T. D. Lee, Phys. Rev. 95, 1329 (1954).

[109] U. Haber-Schaim and W. Thirring, Nuovo cimento 2, 100 (1955).

[110] A. Klein and B. H. McCormick, Phys. Rev. 98, 1428 (1955).

See also reference 125 .

On "non-renormalizable" field theories.

[111] L. N. Cooper, Some notes on non-renormalizable field theory. (To be published.)

[112] R. Arnowitt and S. Deser, Renormalization of derivative coupling theories. (To be published.)

Convergence and other difficulties in renormalized field theories.

[113] L. Van Hove, Academie Royale de Belgique, Bulletin de la Classe des Sciences, 37, 1055 (1951).

[114] ---, Physica 18, 145 (1952).

[115] F. J. Dyson, Phys. Rev. 85, 631 (1952).

[116] Y. Katayama and K. Yamakazi, Prog. Theor. Phys. 7, 601 (1952).

[117] C. A. Hurst, Proc. Roy Soc. (London) A214, 44 (1952).

[118] C. A. Hurst, Proc. Cambridge Phil. Soc. 48, 625 (1952).

[119] A. Petermann, Phys. Rev. 89, 1161 (1953).

[120] R. J. Riddell, Jr., Phys. Rev. 91, 1243 (1953).

[121] W. Thirring, Helv. Phys. Acta 26, 33 (1953).

[122] R. Utiyama, Prog. Theor. Phys. 9, 593 (1953).

Covariant formal theories.

[123] R. P. Feynman, Phys. Rev. 80, 440 (1950).

[124] J. Schwinger, Proc. Natl. Acad. Sci. U.S., 37, 452, 455 (1951).

[125] S. F. Edwards and R. E. Peierls, Proc. Roy. Soc. (London) A224, 24 (1954).

Problems involving several perturbations (selected theoretical).

[126] K. M. Watson, Phys. Rev. 88, 1163 (1952).

[127] H. E. Moses, Phys. Rev. 91, 185 (1953).

[128] E. Gerjuoy, Phys. Rev. 91, 645 (1953).

[129] Y. Fujimoto, S. Hayakawa, and K. Nishijima, Prog. Theor. Phys. 10, 113 (1953).

[130] N. C. Francis and K. M. Watson, Phys. Rev. 93, 313 (1954).

[131] T. Kinoshita and Y. Nambu, Phys. Rev. 94, 598 (1954).

[132] I. P. Grant, Proc. Phys. Soc. (London) 67A, 981 (1954).

[133] R. A. Mapleton, Phys. Rev. 96, 415 (1954).

See also references [24], [30], [145] and [146].

Theory of nuclear reactions.

[134] E. P. Wigner and L. Eisenbud, Phys. Rev. 72, 29 (1947).

[135] T. Teichmann, Phys. Rev. 77, 506 (1950).

[136] V. F. Weisskopf, Helv. Phys. Acta 23, 187 (1950).

[137] J. M. Blatt and V. F. Weisskopf, reference [9], chapter X.

[138] T. Teichmann and E. P. Wigner, Phys. Rev. 87, 123 (1952).

[139] R. G. Thomas, Phys. Rev. 97, 224 (1955).

See also references [24] and [169].

Multiple scattering.

[140] M. Lax, Revs. Modern Phys. 23, 287 (1951).

[141] H. Eckstein, Phys. Rev. 83, 721 (1951).

[142] K. M. Watson, Phys. Rev. 89, 575 (1953).

[143] N. C. Francis and K. M. Watson, Phys. Rev. 92, 291 (1953).

[144] G. Takeda and K. M. Watson, Phys. Rev. 97, 1336 (1953).

[145] K. A. Brueckner and C. A. Levinson, Phys. Rev. 97, 1344 (1955).

[146] ---, Phys. Rev. 97, 1353 (1955).

See also reference [150].

The impulse approximation.

[147] G. F. Chew and M. L. Goldberger, Phys. Rev. 77, 470 (1950).

[148] ---, Phys. Rev. 80, 196 (1950).

[149] --- and G. C. Wick, Phys. Rev. 85, 636 (1952).

[150] --- and M. L. Goldberger, Phys. Rev. 87, 778 (1952).

[151] J. Ashkin and G. C. Wick, Phys. Rev. 85, 686 (1952).

[152] S. T. Epstein, Phys. Rev. 86, 836 (1952).

Time reversal.

[153] E. Wigner, Nachr. Ges. Wiss. Gottingen, Math.-Physik Klasse, p.549 (1932).

[154] S. Watanabe, Revs. Modern Phys. 27, 26, 40, 179 (1955).

See also reference [150], appendix.

Variational methods.

[155] J. W. S. Rayleigh, reference [1], vol. 1, p.109 ff.

[156] L. Hulthèn, The variational principle for continuous spectra, X. Cong. Math. Scand., Copenhagen (1946).

[157] ---, Ark. Math., Ast. Phys. 35A, 1 (1948).

[158] J. M. Blatt and J. D. Jackson, Phys. Rev. 76, 18 (1949).

[159] J. Schwinger, Phys. Rev. 78, 135 (1950).

[160] B. A. Lippmann and J. Schwinger, Phys. Rev. 79, 469 (1950).

[161] W. Kohn, Phys. Rev. 74, 1763 (1948).

[162] ---, Phys. Rev. 84, 495 (1951).

[163] ---, Phys. Rev. 87, 472 (1952).

[164] G. T. di Francia, Phys. Rev. 78, 298 (1950); Nuovo cimento 7, 253 (1950)

[165] M. Cini and L. A. Radicati, Phys. Rev. 80, 300 (1950); Nuovo cimento 7, 905 (1950).

[166] T. Kato, Phys. Rev. 80, 475 (1950).

[167] ---, Prog. Theor. Phys. 10, 653 (1953).

[168] B. L. Moiseiwitsch, Phys. Rev. 82, 753 (1951).

[169] J. L. Jackson, Phys. Rev. 83, 249 (1951).

[170] H. J. Maehly, Helv. Phys. Acta 25, 547 (1952).

[171] ---, Nuovo cimento 8, 466 (1951).

[172] H. Feshbach and S. I. Rubinow, Phys. Rev. 88, 484 (1952).

[173] S. Borowitz and B. Friedman, Phys. Rev. 89, 441 (1953).

[174] S. Altshuler, Phys. Rev. 89, 1278 (1953).

[175] H. E. Moses, Phys. Rev. 92, 817 (1953).

[176] ---, Phys. Rev. 96, 519 (1954).

[177] T. Regge and M. Verde, Nuovo cimento 10, 997 (1953).

[178] T. Kikuta, Prog. Theor. Phys. 10, 653 (1953); 12, 10 (1954).

[179] R. E. B. Makinson and J. S. Turner, Proc. Phys. Soc. (London) 66A, 857 (1953).

[180] L. C. Biedenharn and J. M. Blatt, Phys. Rev. 93, 230 (1954).

[181] G. F. Chew, Phys. Rev. 93, 341 (1954).

[182] S. Altshuler and J. F. Carlson, Phys. Rev. 95, 546 (1954).

[183] S. I. Rubinow, Phys. Rev. 96, 218 (1954); 98, 183 (1955).

[184] L. Cohen, Proc. Phys. Soc. (London) 68A, 419, 425 (1955).

[185] P. M. Morse and H. Feshbach, reference [10], chapter 9.

Construction of a potential from the phase shift.

[186] V. Bargmann, Revs. Modern Phys. 21, 488 (1949).

[187] ——, Phys. Rev. 75, 301 (1949).

[188] R. Jost and W. Kohn, Phys. Rev. 87, 977 (1952); 88, 382 (1952).

[189] B. Holmberg, Nuovo cimento 9, 597 (1952).

[190] N. Levinson, Phys. Rev. 89, 755 (1953).

[191] R. G. Newton and R. Jost, Nuovo cimento 1, 590 (1955).

[192] I. Kay and H. E. Moses, New York University, Institute of Mathematical Sciences, Division of Electromagnetic Research, Research Report No. CX-18 (1955).

Causality and dispersion relations.

[193] H. A. Kramers and W. Heisenberg, Z. Physik 31, 681 (1925).

[194] R. Kronig, Physica 12, 543 (1926).

[195] G. Wentzel, Helv. Phys. Acta 21, 49 (1948).

[196] N. Hu, Phys. Rev. 74, 131 (1948).

[197] W. Schützer and J. Tiomno, Phys. Rev. 83, 249 (1951).

[198] J. S. Toll, thesis, Princeton (1952).

[199] E. P. Wigner, Revista Mexicana de Physica 1, 91 (1952).

[200] J. M. Lozano and F. M. Medina N., Revista Mexicana de Physica 1, 102 (1952).

[201] M. Moshinsky, Revista Mexicana de Physica 1, 117 (1952).

[202] N. G. van Kampen, Revista Mexicana de Physica 2, 233 (1953).

[203] ---, Phys. Rev. 89, 1072 (1953); 91, 1267 (1953).

[204] M. Gell-Mann, M. L. Goldberger, and W. E. Thirring, Phys. Rev. 95, 1612 (1954).

[205] M. L. Goldberger, Phys. Rev. 97, 508 (1955).

[206] E. P. Wigner, Phys. Rev. 98, 145 (1955).

[207] R. Karplus and M. A. Ruderman, Phys. Rev. 98, 771 (1955).

[208] C. J. Goebel, R. Karplus, and M. Ruderman, Momentum dependence of phase shifts. (To be published.)

[209] M. L. Goldberger, Causality conditions and dispersion relations. I. Boson fields. (To be published.)

[210] M. L. Goldberger, H. Miyazawa, and R. Oehme, Application of dispersion relations to pion-nucleon scattering. (To be published.)

Applications of Fredholm theory.

[211] M. Neuman, Phys. Rev. 83, 1258 (1951).

[212] A. Salam and P. T. Matthews, Phys. Rev. 90, 690 (1953).

[213] J. Hamilton, Phys. Rev. 91, 1524 (1953).

[214] I. E. McCarthy and H. S. Green, Proc. Phys. Soc. (London) 67A, 719 (1954).

[215] P. Swan, Phys. Rev. 96, 1144 (1954).

[216] A. Visconti, J. phys. et radium 16, 1 (1955).

Tamm-Dancoff formalism.

No mention of the so-called Tamm-Dancoff method for treating meson-nucleon problems has been made in this article, and accordingly no list of references is given. Unfortunately the operator formalism has often been misused in articles appearing on this subject. Even setting aside the question of the validity of the whole Tamm-Dancoff approach to field theoretical problems, one frequently finds in the literature that insufficient attention has been paid to such things as state-vector normalization, unitarity of transformations, energy dependence of computed potentials, and consistency of orders of approximation. For a discussion of some of these points and a selected bibliography the reader is referred to an article by S. Ôkubo, Prog. Theor. Phys. 12, 603 (1954).