Theory of Time-Dependent Scattering for Multichannel Processes

H. EKSTEIN
Armour Research Foundation of Illinois Institute of Technology, Chicago, Illinois
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The existing time-dependent formal theory of scattering is valid only for the simplest case. The theory is extended to the general case of rearrangement collisions including the case where all or some particles are indistinguishable.

The outstanding feature of the scattering process is the existence of asymptotically constant observables. The formal expression of this fact is the existence of a set of basis functions Φ_n such that, if the Schrödinger state is written as a linear combination $\int c(n,t)\exp(-iE_nt)\Phi_n dn$, the coefficients c have time-independent limits $c_\pm(n)$ for $t=\pm\infty$, the squares of which are observed probabilities. While in the simplest case the Φ_n's are eigenfunctions of the unperturbed Hamiltonian, they form in general a nonorthogonal and linearly not-independent set which can be explicitly given, but there exists no linear operator of which they are eigenfunctions. As a consequence, it is impossible to define an interaction representation in which the states have asymptotic limits, and no linear *S-operator* exists. An *S-matrix* is defined, and it is shown to be connected with cross sections in the usual manner. An expression for the S-matrix in terms of time-independent solutions is given and shown to reduce to the usual one in the simplest case, but not in general. An integral equation for the scattering amplitude is given which is nonlinear. It has, however, the advantage of exhibiting directly the contribution of bound states in addition to Born's approximation. Unitarity and reciprocity relations for the general case are derived.

I. INTRODUCTION

THE general case of scattering, where the reaction products may be different from the colliding systems, has been extensively studied in the time-independent formalism.[1–3] Stueckelberg,[4] Schwinger,[5] and Dyson[6] introduced a representation of the scattering operator as the limit of a time-dependent operator U. This representation is not only satisfactory from a fundamental viewpoint, but also practically advantageous. The time-dependent formalism has since received much attention[7–13] but it has not been generalized sufficiently to describe the general case of rearrangement collisions. The definitions of the S-matrix given by Schwinger and Dyson are not valid for the general case. This limitation seems to have been recognized only by Belinfante and Møller.[13]

The purpose of the present paper is the definition and characterization of the S-matrix as a limit of a time-dependent function for the general case.

Since the time-independent theory cannot only deal with all scattering problems in configuration space, but is also able to produce time-dependent solutions by appropriate linear combinations of steady-state solutions,[14] the present paper does not fulfill a real need in this field. The need for a reformulation arises in field theory, where the use of configuration space is impossible or awkward, and it is in view of this application that the present study was undertaken. In addition, some aspects of the theory in configuration space are more easily accessible in a formulation which is time-dependent at the outset, e.g., the orthogonality of steady-state solutions which describe different entrance channels (Sec. IV).

We start with a re-examination of the basic question: which mathematical expressions represent the observed quantities?

In scattering experiments, the evolution of the wave packet in time is masked by the rapid succession of independent and incoherent scattering events. The time-dependent theory describes only the single scattering event, and not a steady stream of incident particles.

For clarity, a telescoping of these two concepts will be avoided.

The characteristic empirical fact in scattering experiments is that the measured probabilities (differential cross sections) become, for sufficiently large distances, independent of the distance between the region of collision and the location of the measuring device. In the theory of the single event, this must be interpreted as the existence of a limit of observables as time increases. The objects of the theory are these asymptotic constants.

The "initial" information to which these constants are correlated comes from monitoring experiments, in which the incident beam is analyzed after removal of the target. The probability distribution of constants of

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the motion (momenta and internal coordinates) of the free projectile is measured. It is then inferred that in the actual scattering experiment the incident projectiles also have this distribution a long time before they interact with the target, i.e., in the distant past with respect to the time of collision; and even if the incident particles have been released from the source only a short time before their collision, it is useful to think of the incident particle as having traveled an infinite distance before collision. It is unrealistic to assume, as was done in the older literature, that one has in a scattering experiment any information concerning the initial state at a finite time (say, $t=0$). (See Sec. XII.)

The reformulation of scattering theory (by Schwinger and Dyson[5,6]) is not primarily a device to introduce symmetry between past and future, but a step necessary to establish correspondence between measured and calculated quantities.

The purpose of scattering theory is, then, to find the connection between the asymptotic limits of probabilities or probability amplitudes for $t\to+\infty$ and $-\infty$.

In the one-channel case, these amplitudes are the coefficients of the expansion of the Schrödinger wave function in terms of eigenfunctions of the kinetic-energy operator. This is intuitively obvious, and can be shown to be mathematically correct. For the general case, the system of basis functions must be chosen with great care, if the expansion coefficients are to have limits. If the basis system is chosen arbitrarily, i.e., an "unperturbed Hamiltonian" H_0 is arbitrarily separated from the Hamiltonian H, the expansion coefficients will not have limits; if one attempts to use a substitute limit, demonstrably incorrect results are obtained. (See end of Sec. II.)

In scattering experiments, one tries to define the momentum of the incident projectiles as sharply as possible. This has led to the identification of the state in the distant past (or at $t=0$) with a plane wave. The use of a non-normalizable function as a state $\Psi(t)$ leads to mathematical complications[7-9] which are unnecessary. In the present paper, the entire general theory is based on finite wave packets of very general nature. The passage to the limit of sharp initial momentum is made only where the connection between the S-matrix and cross sections in the (idealized) experimental situation is established. (See Sec. XII.)

In Sec. II, the single-channel scattering theory is recapitulated in a somewhat different manner, in order to show its inadequacy for the general case. In Sec. III, a set of basis functions Φ_n is defined such that the Schrödinger state $\Psi(t)$ tends to

$$\Psi(t)\to\int c_{\pm}(n)\exp(-iE_nt)\Phi_n dn$$

for $t=\pm\infty$. In Sec. IV, the S-matrix is defined, expressed in terms of eigenfunctions of the Hamiltonian, and shown to give the usual results in simple cases. In Secs. V and VI, unitarity and reciprocity theorems are derived. In Sec. VII, it is pointed out that no linear operators exist which transform either the state in the distant past into that in the distant future (S-operator) or the set of basis functions into the orthonormal set of "scattering" eigenfunctions $\psi_n^{\pm}$ (Møller's wave operator). Transformation properties of the S-matrix are discussed in Sec. XIII, and two nonlinear integral equations of general validity are derived in Sec. IX. Certain simplifications, which occur when all particles involved are distinguishable, are discussed in Sec. X, and the S-matrix is identified with the coefficients of asymptotic expansion in configuration space in Sec. XI.

The present paper considers only processes which can be described in configuration space. Application to field theory will be made in a later paper.

II. INADEQUACY OF THE ONE-CHANNEL THEORY

The definition of the scattering operator S as the limit of an operator U is, strictly speaking, only applicable to the case of two colliding particles, or, slightly more generally, several particles which are infinitely separated both before and after the collision, as considered by Belinfante and Møller.[13] To show how this one-channel theory is limited, we summarize it in a somewhat modified manner. (We set $\hbar=1$.)

We consider a time-independent Hamiltonian

$$H=W+V, \tag{1}$$

where W is the kinetic energy and V is of limited range. Its positive-energy eigenfunctions are $\psi_{E,s}(x)$:

$$H\psi_{E,s}(x)=E\psi_{E,s}, \tag{2}$$

where s are parameters of degeneracy which may be discrete or continuous, but E has a continuous range. A general state of the system without admixture of negative-energy eigenstates at the time $t=0$ may be represented by the Schrödinger wave function

$$\Psi(0)=\int a(E,s)\psi_{E,s}(x)dEds, \tag{3}$$

where the integration may also mean summation with respect to some parameters s, but not with respect to E. The coefficient $a(E,s)$ is a square-integrable function. The state at some time t is then given by

$$\Psi(t)=\int e^{-iEt}a(E,s)\psi_{E,s}dEds. \tag{4}$$

If

$$\int a(E,s)\psi_{E,s}(x)ds$$

is absolutely integrable for every x (a rather mild requirement), then, by the general properties of Fourier integrals,

$$\lim_{|t|\to\infty}\Psi(t)=0, \tag{4a}$$

and since the range where $V \neq 0$ is limited,

$$\lim_{|t|\to\infty} \int \Psi^*(t) V \Psi(t) dx^3 = 0. \tag{5}$$

In other words, the wave packet $\Psi(t)$ will ultimately be outside of the range of V, and its further development is then described by the differential equation

$$i\partial\Psi/\partial t = W\Psi) \quad |t| \to \infty). \tag{6}$$

Hence,[15]

$$\Psi(t) \to e^{-iWt}\Phi_\pm(x) \quad (t \to \pm\infty), \tag{7}$$

where $\Phi_\pm$ is time-independent. If, therefore, the interaction representation is defined, at all times, by

$$\Phi(t) = e^{iWt}\Psi(t), \tag{8}$$

we are assured that the limit

$$\Phi(\pm\infty) = \Phi_\pm \tag{9}$$

exists and it is at least reasonable to assume that an operator S defined by

$$\Phi_+ = S\Phi_- \tag{10}$$

exists, and that it is the limit of an operator $U(t,\tau)$ defined by

$$\Phi(t) = U(t,\tau)\Phi(\tau). \tag{11}$$

In the general case, however, no single Hermitean operator V can be split from the Hamiltonian H such that the essential Eq. (5) holds. For instance, in the simplest case of exchange scattering, we have a particle 1 incident on a particle 2 bound by a fixed center. The Hamiltonian is

$$H = W_1 + W_2 + V_1 + V_2 + V_{12}, \tag{12}$$

where V_1, V_2, and V_{12} are the potentials between the center and the particles, and between the particles, respectively. For exchange scattering we have then

$$\lim_{t\to-\infty} (V_1 + V_{12})\Psi(t) = 0, \tag{13}$$

but

$$\lim_{t\to+\infty} (V_2 + V_{12})\Psi(t) = 0, \tag{14}$$

for that part of Ψ which describes exchange. Therefore, it is not possible to define an interaction representation such that Eq. (9) holds. Both the forms

$$\Phi_1(t) = e^{i(W_1+W_2+V_2)t}\Psi(t) \tag{15}$$

and

$$\Phi_2(t) = e^{i(W_1+W_2+V_1)t}\Psi(t) \tag{16}$$

will fail to have limits for either $t \to +\infty$ or $-\infty$, so that no operator S can be defined in accordance with Eq. (10).

[15] This description is oversimplified for brevity. The point is that for large times, the bulk of $\Psi(t)$ is of the form (7). Since we need only space-integrals in the following, the omission of V for $|t| \to \infty$ is rigorously correct. A more detailed discussion of the limiting process is given in the Appendix.

The distinction between the cases where $\Phi(\pm\infty)$ exists and where it does not, is not a matter of mathematical subtlety which can be overcome by defining a substitute limit: it is a real physical distinction which leads to different results.

As a consequence, the usual time-dependent theory of the S-matrix fails in the multi-channel case. Consider again the case of exchange scattering. The usual formula (e.g., reference 9) for the differential cross section $i \to j$ is

$$\sigma_{ij} \sim |(\Phi_i, V\psi_j^+)|^2 \delta_{E_i,E_j},$$

where Φ_i is an eigenfunction of the unperturbed, ψ_j^+ one of the total Hamiltonian. In exchange scattering, the particle initially bound is found at large distances from the center of force. This situation must be described by a Φ_i which represents a positive-energy state of the unperturbed system of energy E_p. If the energy E_j is negative, it is clear that no solution of the equation $E_i = E_j$ for such states Φ_i exists. Therefore, the usual formalism would predict no exchange scattering, if taken literally.[16]

III. THE BASIS FUNCTIONS

We consider a time-independent Hamiltonian H in the Schrödinger representation with a number of potential terms. All potentials are assumed to be of limited range. In particular, no Coulomb interaction is considered at this point: long-range forces may be considered as a limiting case.

The division of configuration space into external and internal regions is well known.[1-3] We assume that in the external region at least one term of the Hamiltonian vanishes so that the solution of the time-independent Schrödinger equation in each part of the external region is a superposition of basis functions Φ_n which represent bound fragments not interacting with each other. The channel α is characterized by the vanishing of the interaction term V_α (and no other term). To illustrate this definition, which differs slightly from the usual one, by a simple example, consider a system consisting of two particles and an external field, vanishing outside a region near the origin. In the 6-dimensional configuration space, one can distinguish four channels as follows:

$$|\mathbf{r}_1| \text{ small}, |\mathbf{r}_2| \text{ large}; \quad |\mathbf{r}_2| \text{ small}, |\mathbf{r}_1| \text{ large};$$
$$|\mathbf{r}_1+\mathbf{r}_2| \text{ large}, |\mathbf{r}_1-\mathbf{r}_2| \text{ small};$$
$$|\mathbf{r}_1+\mathbf{r}_2| \text{ and } |\mathbf{r}_1-\mathbf{r}_2| \text{ large}.$$

The definition of channels is only based on geometric relations, and does not include spins or internal coordinates of fragments.

[16] Although this point is rather obvious, it is perhaps not unnecessary to point out the limitations of the usual formalism, because it is frequently considered to be generally valid. Gell-Mann and Goldberger (reference 9) treat several multi-channel cases time-dependently, starting each time from prime principles and obtain correct results. Their S-matrix formalism, however, is restricted to single-channel processes.

The operator

$$H-V_\alpha=H_\alpha \tag{17}$$

may be subdivided into the kinetic energy of the relative motion of the mass centers of fragments, and the Hamiltonian describing the motion of internal coordinates of the fragments. The basis functions are then products of the plane wave functions of the mass centers and of bound-state eigenfunctions of the fragments, if all particles are distinct; if some of the particles are identical, the basis functions are symmetrized or antisymmetrized linear combinations. In the latter case, a basis function Φ_n is finite in all those channels which are obtained by permutation of identical particles in one channel α; in the above example, these are the first and the second channels. The effective Hamiltonians in this group of channels are obtained from Eq. (17) by a permutation operation. We will then say that the basis function Φ_n belongs to a group of channels α. The basis functions Φ_n of one group of channels are not mutually orthogonal, and in either case they are not orthogonal to those of other channels. The basis functions of one group of channels form, in general, an incomplete set, since only bound states of fragments are contained in it; however, the basis functions of the "free" channel (all individual particles noninteracting) form always a complete set by themselves. Thus, the complete set of basis functions is not linearly independent and, of course, not orthonormal. They cannot be considered as eigenfunctions of a Hermitean operator H_0.

While the channels are defined outside the internal region, the basis functions Φ_n are defined everywhere, and their overlap is important. We do not use special solutions for the internal region, as do Wigner and Eisenbud.[1]

In the absence of admixture of bound states of the total system, the arguments of Sec. II show that the entire wave function $\Psi(t)$ will ultimately be in the external region. While Eq. (6) does not hold, we have for the part of Ψ which is contained in channel α

$$i\partial\Psi/\partial t=H_\alpha\Psi \quad (|t|\to\infty), \tag{18}$$

and it is clear from the definition of the basis functions Φ_n that

$$\Psi(t)\to\int c_\pm(n)e^{-iE_nt}\Phi_n dn \quad (t\to\pm\infty), \tag{19}$$

where E_n are the eigenvalues of H_α, H_β, etc., and the integration is meant to include summation over all channels.

While the basis functions are not orthonormal, they have the property that the normalization integral over the total configuration space

$$(\Phi_n,\Phi_m)<\infty \quad (n\neq m). \tag{20}$$

We may assume them to be normalized so that

$$(\Phi_n,\Phi_m)=\delta(n-m)+g(n,m), \tag{21}$$

where $g(n,m)$ is square-integrable and bounded. This leads to the *asymptotic orthogonality* of the basis functions in the following sense:

$$\lim_{t\to\pm\infty}\left(\Phi_n,\int e^{-iE_mt}\Phi_m c_\pm(m)dm\right)$$

$$=c_\pm(n)e^{-iE_nt}+\lim_{t\to\pm\infty}\int e^{-iE_mt}g(n,m)c_\pm(m)dm$$

$$=c_\pm(n)e^{-iE_nt}. \tag{22}$$

The last step follows from the general property of Fourier integrals which has been used already in Sec. II.

As usual, the absolute square of the scalar product

$$(\Phi_{nk\alpha},\Psi(t))$$

is the probability of finding fragments in certain bound states n, with their mass centers having relative momenta $\mathbf{k}_\alpha$. The asymptotic orthogonality of the Φ_n's guarantees that, in spite of the unusual properties of the basis functions, the asymptotic probabilities are just the absolute squares of the coefficients $c_\pm(n)$ in Eq. (19).

IV. S-MATRIX

For $t\to\pm\infty$,

$$e^{-iHt}\Psi(0)\to\int e^{-iE_nt}c_\pm(n)\Phi_n dn. \tag{23}$$

Therefore,

$$\Psi(0)=\lim_{t\to\pm\infty}\int e^{i(H-E_n)t}c_\pm(n)\Phi_n dn. \tag{24}$$

To put this equation into a more useful form, we use the mathematical relation

$$\lim_{t\to\pm\infty}f(t)=\pm\lim_{\epsilon\to+0}\epsilon\int_0^{\pm\infty}\exp(\mp\epsilon t)f(t)dt, \tag{25}$$

which is correct if the limit of $f(t)$ exists.[17] If we set

$$f(t)=e^{iAt}g, \tag{26}$$

where A is a Hermitean operator, and g is time-independent, we get

$$\lim_{t\to\pm\infty}e^{iAt}g=\pm\lim_{\epsilon\to+0}\epsilon\int_0^{\pm\infty}e^{(iA\mp\epsilon)t}gdt$$

$$=\mp\lim_{\epsilon\to+0}\frac{\epsilon}{iA\mp\epsilon}g=\lim_{\epsilon\to+0}[1-(A\pm i\epsilon)^{-1}A]g. \tag{27}$$

[17] This theorem was first used in connection with scattering by Gell-Mann and Goldberger.[9] However, they use the right-hand side of Eq. (25) to define a substitute limit in a case where the proper limit does not exist. In the present paper, the limit exists properly, and Eq. (25) is used merely as a mathematical tool.

By the use of this transformation, Eq. (24) becomes

$$\Psi(0)=\lim_{\epsilon\to+0}\int c_{\pm}(n)\times[1-(H-E_n\pm i\epsilon)^{-1}(H-E_n)]\Phi_n dn. \quad (28)$$

The functions

$$\psi_n{}^{\pm}=\lim_{\epsilon\to+0}[1-(H-E_n\mp i\epsilon)^{-1}(H-E_n)]\Phi_n \quad (29)$$

are solutions of the steady-state Schrödinger equation describing outgoing and ingoing waves, respectively, which are asymptotically equal to Φ_n. Indeed, if we set

$$\psi_n{}^{\pm}=\Phi_n+\psi_{sn}{}^{\pm}, \quad (30)$$

the Schrödinger equation is

$$(H-E_n)\psi_{sn}{}^{\pm}=-(H-E_n)\Phi_n, \quad (31)$$

and

$$\psi_{sn}{}^{\pm}=-\lim_{\epsilon\to+0}(H-E_n\mp i\epsilon)^{-1}(H-E_n)\Phi_n, \quad (32)$$

and Eq. (29) follows.[18]

We shall now prove that the solutions $\psi_n{}^+$ and $\psi_n{}^-$ each form an orthogonal system, even if they belong to different groups of channels.

By comparing Eqs. (24), (28), and (29), we have

$$\lim_{t\to\pm\infty}\int e^{i(H-E_n)t}c_{\pm}(n)\Phi_n dn=\int c_{\pm}(n)\psi_n{}^{\mp}dn, \quad (33)$$

or, symbolically,

$$\lim_{t\to\pm\infty}e^{i(H-E_n)t}\Phi_n=\psi_n{}^{\mp}, \quad (34)$$

although this equation is meaningful only if multiplied by a square integrable $c(n)$ and integrated, and the time limit taken subsequently. Hence,

$$\begin{aligned}\int c(m)(\psi_n{}^{\mp},\psi_m{}^{\mp})dm&=\lim_{t\to\pm\infty}\int c(m)(e^{i(H-E_n)t}\Phi_n,e^{i(H-E_m)t}\Phi_m)dm\\&=\lim\int c(m)e^{-i(E_m-E_n)t}(\Phi_n,\Phi_m)dm\\&=\lim\int c(m)e^{-i(E_m-E_n)t}[\delta(n-m)+g(n,m)]dm\\&=c(n)+\lim\int c(m)e^{i(E_m-E_n)t}g(n,m)dm\\&=c(n). \quad (35)\end{aligned}$$

[18] In the following, the "lim" symbol will frequently be omitted for brevity.

The last two steps follow from Eq. (21) and from the asymptotic vanishing of Fourier transforms of square-integrable functions.

Equation (35) proves the orthonormality of the eigenfunctions $\psi_n{}^+$ and, separately, of the $\psi_n{}^-$.

It should be remembered at this point that the functions $\psi_{n\alpha}{}^{\pm}$ belonging to a group of channels α do not form a complete set, since their asymptotic parts Φ_n include only bound states of the colliding fragments. Therefore, Eq. (35) is not absurd, as it would be if a subset of the $\psi_n{}^+$ were already complete. Nevertheless, the result is surprising: there is at least one channel (the "free" channel) which has already a complete set of Φ_n's. Each of these Φ_n's has an associated ψ_n which nevertheless is orthogonal to all ψ_n's of other channels.

Equations (24) and (33) may be written explicitly

$$\Psi(0)=\int c_-(n)\psi_n{}^+dn=\int c_+(n)\psi_n{}^-dn. \quad (36)$$

The S-matrix consists of the elements of the integral operator which relates the initial packet $c_-(n)$ to the final packet $c_+(n)$. It is shown in Sec. XII that the S-matrix so defined is related to cross sections in the usual manner.

In virtue of the orthogonality of the ψ_n's, we obtain from Eq. (36)

$$c_+(n)=\int(\psi_n{}^-,\psi_m{}^+)c_-(m)dm. \quad (37)$$

Hence,

$$S(n,m)=(\psi_n{}^-,\psi_m{}^+). \quad (38)$$

This result is formally identical with one obtained by Gell-Mann and Goldberger.[9] However, because of the different definition of our ψ_n's, it has different consequences.

The representation of the S-matrix as a double time limit is obtained from Eqs. (34) and (38):

$$S(n,m)=\lim_{\substack{t\to+\infty\\ r\to-\infty}}(e^{i(H-E_n)t}\Phi_n,e^{i(H-E_m)r}\Phi_m). \quad (39)$$

From Eq. (29), we have

$$\psi_n{}^-=\psi_n{}^++[(H-E_n-i\epsilon)^{-1}-(H-E_n+i\epsilon)^{-1}](H-E_n)\Phi_n. \quad (40)$$

From Eq. (38),[19]

[19] The operator H is not in general Hermitean with respect to nonsquared integrable functions. If it were, one could conclude that $((H-E_n)\Phi_n,\psi_m{}^+)=(\Phi_n,(H-E_n)\psi_m{}^+)=0$ on the energy shell since $\psi_m{}^+$ is an eigenfunction of H. However, there is no reason to doubt that the adjoint of $(H-E_n-i\epsilon)^{-1}$ is $(H-E_n-i\epsilon)^{-1}$, as long as ϵ is finite.

$$S(n,m)=(\psi_n^-,\psi_m^+)=(\psi_n^+,\psi_m^+)+([(H-E_n-i\epsilon)^{-1}-(H-E_n+i\epsilon)^{-1}](H-E_n)\Phi_n,\psi_m^+)$$
$$=\delta(n-m)+\left[\frac{1}{E_m-E_n+i\epsilon}-\frac{1}{E_m-E_n-i\epsilon}\right]\times((H-E_n)\Phi_n,\psi_m^+)$$
$$=\delta(n-m)-2\pi i\delta(E_n-E_m)\times((H-E_n)\Phi_n,\psi_m^+). \quad (41)$$

Similarly, by solving Eq. (40) for ψ_n^+ and substituting into Eq. (38):

$$S(n,m)=\delta(n-m)-2\pi i\delta(E_n-E_m)(\psi_n^-,(H-E_m)\Phi_m). \quad (42)$$

In the usual notation,

$$S_{nm}=\delta_{nm}-2\pi i\delta(E_n-E_m)\bar{R}_{nm}, \quad (43)$$

where $\bar{R}$ is defined only on the energy shell $E_n=E_m$. Two matrices $R_{nm}^{\pm}$ can then be defined in general by

$$\begin{aligned}R_{nm}^+&=((H-E_n)\Phi_n,\psi_m^+),\\ R_{nm}^-&=(\psi_n^-,(H-E_m)\Phi_m),\end{aligned} \quad (44)$$

which are equal on the energy shell, but not otherwise.

It can be verified that these results are equivalent to the usual ones if a proper Hermitean scattering potential V exists so that Eq. (5) holds and

$$(H-V-E_n)\Phi_n=0. \quad (45)$$

For then, Eq. (44) gives

$$R_{nm}^+=(V\Phi_n,\psi_m^+)=(\Phi_n,V\psi_m^+), \quad (46)$$

which is the familiar expression.[9] If the particles are distinct, and if α is the entrance channel and β one other channel, we have

$$(H-E_n)\Phi_n^\beta=V_\beta\Phi_n^\beta \quad (47)$$

for a basis function Φ_n^β of channel β, and

$$\psi_n^{+\alpha}=\Phi_n^\alpha-(H-E_n-i\epsilon)^{-1}V_\alpha\Phi_n^\alpha. \quad (48)$$

Hence, by Eqs. (44) and (17),

$$R_{nm}^+=(\Phi_n^\beta,V_\beta\psi_n^{+\alpha}),$$

which is also in agreement with previous work.[9]

Next, we consider two identical particles, one incident, the other initially bound. The Hamiltonian is

$$H=W+V(1)+V(2)+V(12), \quad (12)$$

with $V(12)=V(21)$. The basis functions Φ_n are linear combinations of eigenfunctions of the truncated Hamiltonians

$$\begin{aligned}[W+V(1)-E_n]\chi_n(21)&=0,\\ [W+V(2)-E_n]\chi_n(12)&=0,\end{aligned} \quad (49)$$

namely

$$\Phi_n=(1/\sqrt{2})(\chi_n(12)\pm\chi_n(21)). \quad (50)$$

If we set as a first approximation $\psi_m^+\approx\Phi_m$, we have

$$R_{nm}^+=\tfrac{1}{2}(\{[V(1)+V(12)]\chi_n(12)\pm[V(2)+V(12)]\chi_n(21)\},\{\chi_m(12)\pm\chi_m(21)\})$$
$$=(\chi_n(12),[V(1)+V(12)]\chi_m(12))\pm(\chi_n(21),[V(2)+V(12)]\chi_m(12)), \quad (51)$$

which is identical with Oppenheimer's approximation.[20] It is seen that the formula for R_{nm}^+ contains both the "direct" and "exchange" scattering.

V. UNITARITY

The inverse integral operator $S^{-1}(n,m)$ is evidently defined by solving Eq. (36) for $c_-(n)$:

$$c_-(n)=\int S^{-1}(n,m)c_+(m)dm. \quad (52)$$

Again, we can conclude from the orthogonality of the ψ_n^-:

$$c_-(n)=\int(\psi_n^+,\psi_m^-)c_+(m)dm, \quad (53)$$

so that

$$S^{-1}(n,m)=(\psi_n^+,\psi_m^-), \quad (54)$$

and, by comparison with Eq. (38)

$$S(n,m)=[S^{-1}(m,n)]^*, \quad (55)$$

which proves the unitarity of the S-matrix for the general case.

VI. RECIPROCITY RELATION

We prove the reciprocity relation only for the simplest case, where the Hamiltonian is real. In this case, the bound-state eigenfunctions in the Φ_n's may be considered as real, and the complex conjugate of Φ_n merely has the direction of the momenta reversed. This may be expressed by writing $\Phi_n^*=\Phi_{-n}$. From Eq. (39), we have

$$S(-m,-n)=\lim_{\substack{t\to\infty\\ \tau\to-\infty}}(e^{i(H-E_m)t}\Phi_m^*,e^{i(H-E_n)\tau}\Phi_n^*)$$
$$=\lim_{\substack{t\to\infty\\ \tau\to-\infty}}(e^{i(H-E_n)\tau}\Phi_n^*,e^{i(H-E_m)t}\Phi_m^*)^*$$
$$=\lim_{\substack{t\to\infty\\ \tau\to-\infty}}(e^{-i(H-E_n)\tau}\Phi_n,e^{-i(H-E_m)t}\Phi_m)$$
$$=\lim_{\substack{t\to-\infty\\ \tau\to\infty}}(e^{-i(H-E_n)\tau}\Phi_n,e^{i(H-E_m)t}\Phi_m)$$
$$=S(n,m). \quad (56)$$

VII. NONEXISTENCE OF AN S-OPERATOR

If it were possible to define a linear operator H_0 so that

$$H_0\Phi_n=E_n\Phi_n, \quad (57)$$

[20] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (The Clarendon Press, Oxford, 1949).

the asymptotic form of the Schrödinger wave functions could be written

$$\Psi(t)\rightarrow\int e^{-iE_nt}c_{\pm}(n)\Phi_n dn=e^{-iH_0t}\Phi_{\pm}, \tag{58}$$

and an operator S could be defined by

$$\Phi_+=S\Phi_-, \tag{59}$$

as in the single-channel case. Since, however, the set of Φ_n's is not linearly independent, a given basis function Φ_1 may be represented as a linear combination of others

$$\Phi_1=\int a(n)\Phi_n dn, \tag{60}$$

and if H_0 were a linear operator, it would follow that

$$H_0\Phi_1=\int E(n)a(n)\Phi_n dn, \tag{61}$$

which is in general not compatible with

$$H_0\Phi_1=E_1\Phi_1. \tag{62}$$

Consider as an example a basis function Φ_n which represents a bound state of all but one particle and the remaining particle with small kinetic energy so that E_1 is negative. Φ_1 can be represented as a linear combination of the "free" channel functions $\Phi_n{}^f$ which are just products of plane waves and form a complete orthonormal set by themselves:

$$\Phi_1=\int(\Phi_n{}^f,\Phi_1)\Phi_n{}^f dn, \tag{63}$$

and if H_0 were a linear operator,

$$H_0\Phi_1=\int E_n{}^f(\Phi_n{}^f,\Phi_1)\Phi_n{}^f dn, \tag{64}$$

whereas by the definition of H_0,

$$H_0\Phi_1=E_1\int(\Phi_n{}^f,\Phi_1)\Phi_n{}^f dn. \tag{65}$$

Since these two expressions should hold for every point of configuration space, we may conclude from the uniqueness of Fourier integrals that they are incompatible. Hence, no linear operator H_0 can be defined, and therefore neither can any operator S in the usual sense (i.e., no one-to-one association of one dense set of state vectors to another one). It is also impossible to define, in the general case, a linear wave operator Ω through

$$\psi_n{}^+=\Omega\Phi_n. \tag{66}$$

As a proof, consider again the representation of the basis function Φ_1 with negative energy E_1 by plane wave functions $\Phi_n{}^f$. If a linear operator existed, we could conclude

$$\psi_1{}^+=\int(\Phi_n{}^f,\Phi_1)\Omega\Phi_n{}^f dn=\int(\Phi_n{}^f,\Phi_1)\psi_n{}^{+f}dn. \tag{67}$$

However, we have shown that all $\psi_n{}^+$'s are mutually orthogonal; hence the linear combination of $\psi_n{}^{+f}$ must be orthogonal to $\psi_1{}^+$, contrary to the above conclusion. Therefore the continuous matrix $S(n,m)$ must be considered simply as an array of numbers rather than, as in the single-channel case, a particular representation of a linear operator defined in Hilbert space.

VIII. TRANSFORMATION OF THE S-MATRIX

It is not possible to make use of the general transformation theory of linear operators as in the single-channel case. Nevertheless, the usual transformations can be carried out without difficulty. First, the choice of the basis functions Φ_n is sufficiently arbitrary so that linear combinations of degenerate Φ_n's can be formed to obtain functions which are eigenfunctions of the total spin, isotopic spin, etc. Second, the R-matrix which is a function of two sets of momenta may be represented as a sum of spherical waves with respect to both variables: one only has to expand both Φ_n and $\psi_m{}^{\pm}$ and carry out the integrations. In this manner, one obtains the usual discrete matrix elements S_{nm}, well known in the time-independent theory.

However, it is not possible to use spherical waves at the outset of the theory. Time-independent functions which represent outgoing or incoming waves are singular at the origin and therefore not useful as basis functions. Standing spherical waves lack the property that packets of the form

$$\Psi(t)=\int c(n)\Phi_n e^{-iE_nt}dn$$

become (and remain) asymptotically solutions of the Schrödinger equation, since a part of a packet of standing waves will ultimately flow back to the origin. Hence, only functions of the plane-wave type are acceptable basis functions.

IX. INTEGRAL EQUATIONS

We have defined two matrices $R^{\pm}(m,n)$ which are equal on the energy shell $E_m=E_n$, but not otherwise. We shall now obtain integral equations for these matrices.

If in the equation defining $\psi_n{}^+$ [Eq. (29)]

$$\psi_n{}^+=\Phi_n-(H-E_n-i\epsilon)^{-1}(H-E_n)\Phi_n, \tag{68}$$

each term is premultiplied by $(H-E_m)\Phi_m$, one obtains

$$((H-E_m)\Phi_m,\psi_n{}^+)=((H-E_m)\Phi_m,\Phi_n)-((H-E_m)\Phi_m,(H-E_n-i\epsilon)^{-1}(H-E_n)\Phi_n). \tag{69}$$

We now assume that the rigorous eigenfunctions ψ_n^+, together with negative-energy solutions ψ_b (bound states of the total system) form a complete set and we represent the function $(H-E_n)\Phi_n$ as a series of these. Using the definition [Eq. (44)] of R^+, we obtain the integral equation

$$R^+(m,n)=((H-E_m)\Phi_m,\Phi_n)-\int\frac{R^+(ml)R^{+*}(nl)}{E(l)-E(n)-i\epsilon}dl$$
$$+\sum_b\frac{((H-E_m)\Phi_m,\psi_b)((H-E_n)\Phi_n,\psi_b)^*}{E_n+|E_b|}. \quad (70)$$

In the last term, the transition to the limit $\epsilon=0$ can be carried out since all E_b's are negative.

Similarly, one obtains the integral equation for R^-:

$$R^-(mn)=(\Phi_m,(H-E_n)\Phi_n)-\int\frac{R^-(ln)R^{-*}(lm)}{E(l)-E(m)-i\epsilon}dl$$
$$+\sum_b\frac{((H-E_n)\Phi_n,\psi_b)^*((H-E_m)\Phi_m,\psi_b)}{E_m+|E_b|}. \quad (71)$$

These integral equations have the great disadvantage of being nonlinear. The impossibility of finding linear integral equations in the general case seems to be connected with the nonexistence of a proper scattering potential V.[21]

Iteration of the integral equations leads to results quite similar to those of the usual perturbation theory. If we set

$$((H-E_m)\Phi_m,\Phi_n)=V(mn), \quad (72)$$

(although there exists no linear operator of which $V(mn)$ is the matrix element), the two expansions are, in absence of bound states,

$$R^+(mn)=V(mn)-\int\frac{V(ml)V^*(nl)}{E(l)-E(n)-i\epsilon}dl+\cdots, \quad (73)$$

$$R^-(mn)=V^*(nm)-\int\frac{V(ml)V^*(nl)}{E(l)-E(m)-i\epsilon}dl+\cdots. \quad (74)$$

Since[22]

$$V^*(n,m)=(\Phi_n,(H-E_m)\Phi_m)=((H-E_m)\Phi_n,\Phi_m) \quad (75)$$

is equal to $V(mn)$ on the energy shell, the two expansions are equivalent.

The third term in Eqs. (70) and (71) can be evaluated explicitly and could be considered as a correction to the first term which is Born's approximation: whether it is of practical value remains to be seen.

X. DISTINGUISHABLE PARTICLES

If all particles are distinguishable, certain simplifications are possible. The basis functions $\Phi_{n\alpha}$ are then eigenfunctions of H_α [Eq. (17)]. That part of the wave function which is in channel α has the asymptotic form

$$e^{-iH_\alpha t}\psi_{\alpha\pm}(x),$$

where $\psi_{\alpha\pm}$ is time-independent. For the present case, bound states of the total system, ψ_b, may also be considered without additional complication. The total wave function has the asymptotic form

$$\Psi(x,t)\underset{t\to\pm\infty}{\longrightarrow}\sum_\alpha e^{-iH_\alpha(t-t_0)}\psi_{\alpha\pm}(x)+\sum_b e^{-iH(t-t_0)}\psi_b. \quad (76)$$

The states ψ_b vanish exponentially in the external region, and are asymptotically nonoverlapping with the wave packets of the channels. Hence they may be included as an additional channel b, with $H_b=H$:

$$\Psi(x,t)\underset{t\to\pm\infty}{\longrightarrow}\sum_\alpha e^{-iH_\alpha(t-t_0)}\psi_{\alpha\pm}(x). \quad (77)$$

Clearly, $\psi_{b+}=\psi_{b-}$.

Let P_α be a projection operator which annuls the wave function everywhere except in the channel α. Then,

$$P_\alpha\Psi\underset{t\to\pm\infty}{\longrightarrow}\exp[-iH_\alpha(t-t_0)]\psi_{\alpha\pm}(x). \quad (78)$$

We define operators U_α by

$$U_\alpha(t,t_0)=e^{iH_\alpha(t-t_0)}P_\alpha e^{-iH(t-t_0)}. \quad (79)$$

Since $\Psi(t)=e^{-iH(t-t_0)}\Psi(t_0)$, it follows from Eq. (78) that

$$\lim_{t\to\pm\infty}U_\alpha(t,t_0)\Psi(t_0)=\psi_{\alpha\pm}(x), \quad (80)$$

and the limit exists under the indicated conditions. In general,

$$U_\alpha(\pm\infty,t_0)=\lim_{t\to\pm\infty}\exp[iH_\alpha(t-t_0)]P_\alpha$$
$$\times\exp[-iH(t-t_0)]. \quad (81)$$

Since the projection operators P_α cover nonoverlapping parts of the wave function for $t\to\pm\infty$,

$$\lim_{t\to\pm\infty}(P_\alpha\Psi,P_\beta\Psi)=0 \quad (\alpha\neq\beta). \quad (82)$$

Hence, the constancy of the normalization (Ψ,Ψ) requires that

$$\lim_{t\to\pm\infty}\sum_\alpha(P_\alpha\Psi,P_\alpha\Psi)=(\Psi(t_0),\Psi(t_0))=\sum_\alpha(\psi_{\alpha\pm},\psi_{\alpha\pm}). \quad (83)$$

It follows from Eq. (80) that

$$\sum_\alpha U_\alpha^\dagger(\pm\infty,t_0)U_\alpha(\pm\infty,t_0)=1, \quad (84)$$

[21] *Note added in proof.*—If the functions Φ_n were eigenfunctions of a linear operator H_0, Eq. (70) would reduce to Eq. (5.14) of reference 9. For the scattering of mesons by a fixed nucleon, Eq. (71) is identical with Eq. (5.36) of G. C. Wick [Revs. Modern Phys. **27**, 339 (1955)], where Φ is defined by Wick's equation (5.23) and use is made of Eq. (5.28).

[22] It is easy to verify the self-adjoint property of $(H-E_n)$ with respect to the functions Φ_n and Φ_m, from their definition in coordinate space, by Green's theorem.

and

$$\psi_{\alpha\pm}=U_\alpha(\pm\infty,t_0)\Psi(t_0)$$
$$=U_\alpha(\pm\infty,t_0)\textstyle\sum_\alpha U_\alpha^\dagger(\pm\infty,t_0)\psi_{\alpha\pm}. \quad (85)$$

For the single-channel case, these equations reduce to

$$U^\dagger U=UU^\dagger=1, \quad (86)$$

which expresses the unitarity of the U-operator. The operators $U_\alpha^\dagger(\pm\infty,t_0)$ have meaning only when they act on wave packets ψ_α, i.e., on square-integrable wave packets of channel eigenfunctions (α), as can be seen from Eqs. (84) and (86).

In order to relate the state of the distant future to that of the distant past, we observe that, by Eqs. (80), (84), and (81),

$$\psi_{\alpha+}=U_\alpha(\infty,0)\Psi(0)=U_\alpha(\infty,0)\textstyle\sum_\beta U_\beta^\dagger(-\infty,0)\psi_{\beta-}$$
$$=\lim_{\substack{t\to\infty\\ \tau=-\infty}}\textstyle\sum_\beta e^{iH_\alpha t}P_\alpha e^{-iH(t-\tau)}P_\beta e^{-iH_\beta\tau}\psi_{\beta-}. \quad (87)$$

Since each of the operators $e^{-iH_\beta\tau}$ acts only on a wave packet of channel functions (β), the resultant function will still be in the same channel, so that the operator P_β may be omitted.

We define operators

$$S_{\alpha\beta}=U_\alpha(\infty,0)U_\beta^\dagger(-\infty,0), \quad (88)$$

with domains restricted in the foregoing sense. Then,

$$\psi_{\alpha+}=\textstyle\sum_\beta S_{\alpha\beta}\psi_{\beta-}. \quad (89)$$

The constancy of the normalization requires again that

$$\textstyle\sum_\alpha(\psi_{\alpha-},\psi_{\alpha-})=\sum_\alpha(\psi_{\alpha+},\psi_{\alpha+}), \quad (90)$$

and, hence

$$\textstyle\sum_\alpha S_{\alpha\beta}^\dagger S_{\alpha\gamma}=1, \quad (91)$$

if the unit operator is meant only to reproduce wave packets of channel eigenfunctions (γ). By interchanging $+$ and $-$ signs in Eq. (87) and in view of Eq. (88) we have

$$\psi_{\alpha-}=\textstyle\sum_\beta S_{\beta\alpha}^\dagger\psi_{\beta+}, \quad (92)$$

and constant normalization requires that

$$\textstyle\sum_\alpha S_{\gamma\alpha}S_{\beta\alpha}^\dagger=1, \quad (93)$$

with respect to any wave packet of channel eigenfunctions (β).

Let us summarize the results: the state in the distant past (future) is completely specified by the sets of functions $\psi_{\alpha-}(\psi_{\alpha+})$. Each function $\psi_{\alpha\pm}$ is a square-integrable wave packet of channel eigenfunctions (α); they are not mutually orthogonal. The connection between past and future is given by a square array of operators $S_{\alpha\beta}$ by the scheme:

$$\begin{pmatrix}\psi_{1+}\\ \psi_{2+}\\ \cdot\\ \cdot\\ \cdot\end{pmatrix}=\begin{pmatrix}S_{11} & S_{12} & \cdots\\ S_{21} & S_{22} & \\ \cdot & & \cdot\\ \cdot & & \cdot\\ \cdot & & \cdot\end{pmatrix}\begin{pmatrix}\psi_{1-}\\ \psi_{2-}\\ \cdot\\ \cdot\\ \cdot\end{pmatrix} \quad (94)$$

if the functions $\psi_{\alpha+}(\psi_{\alpha-})$ are considered as vector components and the operator array acts in the sense of matrix multiplication. The inverse to Eq. (94) is

$$\begin{pmatrix}\psi_{1-}\\ \psi_{2-}\\ \cdot\\ \cdot\\ \cdot\end{pmatrix}=\begin{pmatrix}S_{11}^\dagger & S_{21}^\dagger & \cdots\\ S_{12}^\dagger & S_{22}^\dagger & \cdots\\ \cdot & & \cdot\\ \cdot & & \cdot\\ \cdot & & \cdot\end{pmatrix}\begin{pmatrix}\psi_{1+}\\ \psi_{2+}\\ \cdot\\ \cdot\\ \cdot\end{pmatrix}. \quad (95)$$

While none of the operators $S_{\alpha\beta}$ is unitary, the array of the $S_{\alpha\beta}$ is unitary in a somewhat extended sense of the word.

The general case of indistinguishable particles can be reduced to that considered here, if it is postulated that the wave packet $\psi_{\alpha-}$ should be equal (or the negative of) any $\psi_{\alpha'-}$, which corresponds, in configuration space, to the interchange of any two particle coordinates. This is the analog of the usual procedure in the time-independent formalism.[20]

XI. IDENTIFICATION WITH HEISENBERG'S S-MATRIX

In the case of distinguishable particles, the R-matrix obtained from time-dependent theory can be connected with the asymptotic form of the time-independent solutions ψ_n^+ in configuration space. Consider a channel α which corresponds to the free motion of N fragments, with mass centers $\mathbf{r}_1\cdots\mathbf{r}_N$. The interaction term V_α vanishes if all relative distances $(\mathbf{r}_1-\mathbf{r}_2)\cdots$ are sufficiently large. The Schrödinger equation for ψ_β^+ may be written

$$(H_\alpha-E)\psi_\beta^+=-V_\alpha\psi_\beta^+, \quad (96)$$

where β is the "entrance channel," i.e., ψ_β^+ has the asymptotic form Φ_β. In channel α, Eq. (96) yields

$$\psi_\beta^+=-(H_\alpha-E-i\epsilon)^{-1}V_\alpha\psi_\beta^++\delta_{\alpha\beta}\Phi_\beta. \quad (97)$$

Equation (97) is now written in that representation which diagonalizes the momenta of the fragments, $\mathbf{k}_1\cdots\mathbf{k}_N$ and the internal energies of the fragments, i.e.,

$$\psi_\beta^+=\textstyle\sum g_l(\mathbf{k}_1\cdots\mathbf{k}_N)\chi_l(\tau),$$

where the functions χ_l are products of bound-state eigenfunctions of the internal Hamiltonians.

$$g_l=\delta_{\alpha\beta}(\mathbf{k}-\mathbf{k}')-\sum_1^N[W(\mathbf{k}_n)-E_l-i\epsilon]^{-1}V_\alpha\psi_\beta^+. \quad (98)$$

The remainder of the calculation is identical with the one in the single-channel case[23] except that several momenta $\mathbf{k}$ and coordinates $\mathbf{r}'$ are involved. One transforms g_l into coordinate representation by Fourier integrations, going to the limit of large $\mathbf{r}_n$ and large relative distances $(\mathbf{r}_1-\mathbf{r}_2)\cdots$. The result is a product of Green's functions of the individual fragments with a coefficient

$$(\Phi_\alpha,V_\alpha\psi_\beta^+)=R^+(n_\alpha m_\beta),$$

[23] P. A. M. Dirac, *The Principles of Quantum Mechanics* (The Clarendon Press, Oxford, 1947), third edition, p. 196.

where Φ_α corresponds to those momentum vectors which point toward the location of the fragments (i.e., $\mathbf{k}_1 \| \mathbf{r}_1$, etc.).

This identification of the matrix R with the asymptotic form of the time-independent solution is valid only for identifiable particles. For the general case, the connection is complicated, as can be seen from the exchange scattering considered in Sec. IV. We obtained there the direct and exchange scattering amplitudes together from the general formalism, but we would have to add up contributions from two essentially different parts of configuration space if we wanted to obtain the observable cross sections from the time-independent solutions. The only possibility for using time-independent formalism is to disregard the identity of the particles at first and to make the necessary corrections subsequently, as it is done usually.[20] In field theory, such a procedure would be extremely awkward, if at all feasible. Thus, the only reliable foundation for scattering in field theory is the time-dependent approach. This was the main motivation for the present investigation.

XII. CROSS SECTIONS

In scattering, the question is not that usually considered: given the state at an initial time, what are probabilities at a later time? It is rather: given that the state at a time (say, zero) is known when the target is removed to infinity, what are probabilities at times $t \to \infty$ when the target is returned to its place (say, $\mathbf{x}=0$)? The data obtained in the monitoring experiment can be evaluated as follows: If it is known that a wave packet is described by

$$\Psi(t)=\int c(n)\Phi_n e^{-iE_n t}dn, \tag{99}$$

for all times at which the target is sufficiently far from the projectile, then the monitoring experiments provide information (partial or complete) on $c(n)$, since

$$\Psi(0)=\int c(n)\Phi_n dn, \tag{100}$$

after removal of the target. When the target is restored, Eq. (100) does not hold, but $\Psi(t)$ is still described by Eq. (99) for $t \to -\infty$, when the projectile is far removed from the target. Hence, the monitoring data describe the function $c_-(n)$.

The particular form of $c_-(n)$ usually considered (and from which the more general case can be handled by linear superposition) is that for which c_- describes a state in which the internal coordinates are characterized by sharp discrete quantum numbers, while the momentum $\mathbf{k}$ of the projectile is almost sharp. Suppose that, in the monitoring experiment, the wave function was found to have the form of a plane wave with propagation vector $k_{0z}=K_0$ inside a large box of edge a, and to vanish outside. We can then infer that in the scattering experiment

$$c_-(\mathbf{k},n)=\left(\frac{2}{\pi a}\right)^{\frac{3}{2}}\frac{\sin(ak_x/2)}{k_x}\frac{\sin(ak_y/2)}{k_y}\times\frac{\sin[a(k_z-K_0)/2]}{k_z-K_0}\delta_{nn_0}, \tag{101}$$

where c_- has been normalized as usual, and n stands for all discrete subscripts of Φ_n. Let

$$\delta_a(x)=\frac{1}{\pi}\frac{\sin(ax/2)}{x} \tag{102}$$

and

$$\Delta_a(x)=\left(\frac{2}{\pi a}\right)^{\frac{1}{2}}\frac{\sin(ax/2)}{x}, \tag{103}$$

so that

$$\lim_{a\to\infty}\delta_a=\delta(x) \tag{104}$$

and

$$\lim_{a\to\infty}(\Delta_a)^2=\delta(x). \tag{105}$$

The asymptotic probability density for finding the system characterized by momenta $\mathbf{k}$ and discrete labels n, is

$$P(\mathbf{k},n)=\left|\sum_{n'}\int(\mathbf{k}n|S|\mathbf{k}'n')c_-(\mathbf{k}'n')d\mathbf{k}'\right|^2. \tag{106}$$

If a were taken to the limit now, the result would show no scattering because a projectile spread over all space has a vanishing chance of hitting a finite target.[24] We are interested in the number $N(\mathbf{k},n)$ of measurements if the current density j of projectiles is given. Clearly, the number of incident particles per second is

$$n=a^2 j, \tag{107}$$

and, hence,

$$N=a^2 jtP. \tag{108}$$

It is now possible to let a increase, j being fixed. The number of measurements $(\mathbf{k},n)$ per interval $d\mathbf{k}$ and per second is

$$\frac{N}{t}=j\lim_{a\to\infty}\left|\sum_{n'}\int a(\mathbf{k}n|S|\mathbf{k}'n')c_-(\mathbf{k}'n')d\mathbf{k}'\right|^2, \tag{109}$$

[24] This is due to the fact that we use no box to define the basis functions. The fact that in an idealized scattering experiment, the probabilities vanish and the cross section appears as an alternative to (rather than proportional to) the probability, is pointed out by W. Heitler, *The Quantum Theory of Radiation* (The Clarendon Press, Oxford, 1954), third edition.

or, by Eqs. (101–103),

$$\frac{N}{t}=j\lim_{a\to\infty}\left|2\pi\int d\mathbf{k}'(\mathbf{k}n|S|\mathbf{k}'n_0)\times\delta_a(k_x')\delta_a(k_y')\Delta_a(k_z'-K_0)\right|^2. \quad (110)$$

If the two functions δ_a are first taken to the limit, the integral gives, by Eq. (43), for $\mathbf{k}'\neq k_0$,

$$-2\pi i(\mathbf{k}n|R|p_0n_0)(dp/dE_0)\Delta_a(p_0-K_0),$$

where E_0 is the energy of the initial Φ as a function of momentum p, and p_0 is that momentum which satisfies $E_{\text{final}}=E_0(p)$. After squaring, Δ_a is taken to the limit:

$$\frac{N}{t}=(2\pi)^4j|(\mathbf{k}n|R|p_0n_0)|^2\left(\frac{dp}{dE_0}\right)^2\delta(p_0-K_0)$$

$$=(2\pi)^4j|R_{f0}|^2\left(\frac{dp}{dE_0}\right)^2\frac{dE_0}{dp}\delta(E_f-E_0). \quad (111)$$

The differential cross section is

$$d\sigma=\frac{d\Omega}{jt}\int Nk^2dk$$

$$=(2\pi)^4d\Omega\int|R_{f0}|^2\frac{dp}{dE_0}k^2\frac{dk}{dE_f}\delta(E_f-E_0)dE_f$$

$$=(2\pi)^4d\Omega|R_{f0}|^2\frac{dp}{dE_0}\frac{dk}{dE_f}k_f^2, \quad (112)$$

where R_{f0} and the other factors are taken on the energy shell. Although we have used units $\hbar=1$, Eq. (112) is also correct in cgs units if p and k are considered as propagation vectors rather than momenta. Equation (112) can be written in terms of final and initial momenta and velocities p_f, v_i, v_f in the more familiar form

$$d\sigma=(2\pi/\hbar)^4d\Omega|R_{fi}|^2(p_f^2/v_iv_f). \quad (113)$$

It has now been shown that the S-matrix defined in Sec. IV has the same relationship to cross sections as the S-matrix usually defined for the single-channel case.

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APPENDIX

In the following, we distinguish between strong and weak convergence of asymptotic limits. From

$$\lim_{|t|\to\infty}\Psi(t)=0, \quad (A1)$$

it follows that $(\Psi(t),V\Psi(t))$ vanishes asymptotically, but, of course, not that (Ψ,Ψ) or $(\Psi,W\Psi)$ vanish. The equation

$$\lim_{|t|\to\infty}V\Psi(t)=0 \quad (A2)$$

holds in the strong sense, i.e., it can be formally multiplied by a bounded function, integrated over space, and the time limit taken subsequently while (A1) holds only in the weak sense. To avoid confusion, all equations involving time limits of functions, except (4a), are meant to hold in the strong sense. To summarize the notation explicitly, Eq. (A2) is an abbreviation for

$$\lim_{t\to\infty}(f,V\Psi(t))=0, \quad (A3)$$

where $\Psi(t)$ is a solution of the time-dependent Schrödinger equation, square integrable, and containing no admixture of eigenstates of the total Hamiltonian which belong to the discrete spectrum, and f is a bounded function, not necessarily square integrable.

A more precise mathematical discussion is found in reference 12. The possibility of including admixtures of discrete-state eigenfunctions is discussed in reference 10.