The P-wave scattering length $a_{33}=0.225$ is reasonably close to the value $a_{33}=0.235$ given by Orear[12] as the one which fits the slope at low energies. The value of a_{31} and a_{13} are small and negative as expected. However, the value of a_{11} is much too large.

We estimated the changes that would occur if the value of $f^2=0.1$ were reduced to $f^2=0.08$. The magnitudes of δ_1 and δ_3 both increase. The effect of D waves decreases in magnitude but still increases the magnitudes of both δ_1 and δ_3. The P-wave scattering lengths decrease to $a_{33}=0.20$, $a_{31}=a_{13}=-0.042$, and $a_{11}=-0.13$, respectively. In other words, the qualitative behavior of the quantities above is unchanged.

The present study indicates that relativistic dispersion relations with the assumption of the dominance of the (3,3) resonance reproduces the experimental energy dependence of the S-wave phase shifts and the P-wave scattering lengths reasonably well.

ACKNOWLEDGMENT

The author is grateful to Professor G. F. Chew for a series of preprints which were very helpful.

PHYSICAL REVIEW VOLUME 108, NUMBER 6 DECEMBER 15, 1957

Modified Plane Waves and Rearrangement Collisions*

M. N. Hack
Argonne National Laboratory, Lemont, Illinois
(Received April 15, 1957; revised manuscript received July 8, 1957)

The use of modified plane waves as initial- or final-state basis vectors in the calculation of transition amplitudes for scattering problems is justified in a general manner by time-dependent and time-independent methods. Expressions for the S matrix in terms of modified plane waves are derived for rearrangement collisions. An equivalence theorem is obtained, by means of which the S matrix can be expressed in a variety of alternative forms.

I. INTRODUCTION

In the quantum-mechanical calculation of transition amplitudes for scattering problems by means of modified plane waves, a question arises concerning the appropriate choice of continuum eigenfunctions for describing ultimately free particles. This question occurs already in the familiar case of ionization collisions where it is well known that the correct choice of modified plane wave for describing an ionized particle is the ingoing-wave continuum eigenfunction.[1] Another well-known example is scattering by two potentials where modified plane waves are used in order to take advantage of the fact that the wave function could be calculated exactly or to a good approximation if only one of the potentials were acting. Problems of this type have caused some difficulty in the past.[2]

An interesting physical discussion of the reason for the occurrence of the ingoing-wave basis vectors for final states of unbound particles has been given by Breit and Bethe.[3] The essential point is the fact that it is the *ingoing-wave* solutions which merge with plane-wave solutions at the time $t=+\infty$ at which the measurement of the scattering is regarded as being made. An elegant formal derivation, without approximation and encompassing the case of explicitly time-dependent interactions, has been given by Altshuler.[4] Altshuler's treatment is applicable to ionization collisions, but not to scattering by two potentials, since he omits the term in the transition amplitude arising from the inhomogeneous term of the integral equation for the scattering wave function. On the other hand, a treatment given by Park[5] is applicable to the example of scattering by two potentials, but not to ionization, since he starts from the matrix element for plane waves and assumes that eigenfunctions of the same free Hamiltonian describe both initial and final states. Three examples, including examples of the two types mentioned above, as well as the case of a pickup process, have been treated by Gell-Mann and Goldberger.[6] In each case Gell-Mann and Goldberger have recourse, for justification of the expression for the transition rate for true plane waves from which they start, to a time-dependent theory which is unfortunately unnecessarily cumbersome and somewhat obscure from the physical point of view. No treatment has been given up to now which is applicable to general rearrangement collisions.

The present paper aims to fill this gap and to provide a general justification of the use of modified plane waves on the basis of methods of the formal theory of

---

* Work performed under the auspices of the U. S. Atomic Energy Commission.

[1] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, New York, 1949).

[2] Bethe, Maximon, and Low, Phys. Rev. **91**, 417 (1953).

[3] G. Breit and H. A. Bethe, Phys. Rev. **93**, 888 (1954). This paper contains references to earlier treatments of particular cases.

[4] S. Altshuler, Nuovo cimento **3**, 246 (1956).

[5] D. Park, Nuovo cimento **3**, 979 (1956). See also the treatment of the case of scattering by two potentials given by B. A. Lippmann, Ann. Phys. **1**, 113 (1957).

[6] M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953).

scattering. In Secs. II and III we treat, by time-dependent and time-independent methods respectively, a class of problems which includes as special cases the examples of ionization and scattering by two potentials mentioned above. In Sec. IV we treat rearrangement collisions on a general basis and obtain new expressions for the S matrix in terms of modified plane waves. An equivalence theorem is obtained, which provides a large class of alternative expressions for the S matrix. It may be expected that this theorem will prove useful in applications since it provides a variety of alternative bases for the start of approximation calculations of scattering amplitudes.

Concerning terminology and assumptions, we make the following remarks. The S-matrix element for a given scattering process is determined by specifying the total Hamiltonian H, the total energy E, and the initial- and final-state basis vectors. By plane wave basis vector we mean a non-normalizable eigenfunction, of a self-adjoint operator K, such that all ultimately free particles are described by plane wave functions. The operator K is called a "free Hamiltonian." If bound particles are present, the plane-wave basis vectors will also contain bound-state eigenfunctions, so that the free Hamiltonian in general contains interactions as well as kinetic energy operators. By "unperturbed Hamiltonian" we mean a self-adjoint operator H_0 which may differ from the initial- or final-state free Hamiltonian, or both, by including additional interactions such that some or all of the plane-wave functions are replaced by asymptotically equivalent ingoing- or outgoing-wave continuum eigenfunctions. All interactions are assumed to vanish sufficiently strongly as the particles become infinitely distant from each other and from external regions of force. Eigenfunctions of unperturbed Hamiltonians which correspond to those of free Hamiltonians by having plane waves replaced by asymptotically equivalent ingoing- or outgoing-wave continuum eigenfunctions are called "modified plane wave" basis vectors. We shall only be concerned with modified plane-wave basis vectors in which the continuum eigenfunctions are all of the same type, either ingoing or outgoing; basis vectors in which some of the continuum eigenfunctions are ingoing and some outgoing will not occur. The definition of (true) plane-wave basis vector employed here is, apart from modifications in the case of indistinguishable particles, the same as that adopted in a recent paper on multichannel scattering theory by Ekstein.[7] The treatment given here will be confined to distinguishable particles.

II. TIME-DEPENDENT THEORY

In this section we consider the case where the initial- and final-state basis vectors are eigenfunctions of the same unperturbed Hamiltonian H_0.

The time-dependent scattering wave function $\psi(t)$ which develops out of the initial state vector $\chi(t)$ is given by the explicit formula

$$\psi(t)=\chi(t)+\frac{1}{i}\int_{-\infty}^{t} e^{-iH(t-\tau)}V\chi(\tau)d\tau. \tag{1}$$

Here units are chosen such that $\hbar=1$, and the total Hamiltonian H and the unperturbed Hamiltonian $H_0=H-V$ are time-independent self-adjoint operators. The first term of Eq. (1) describes the time development of the initial state vector, representing a wave packet of primary particles incident on the scattering system, as if the interaction V were absent. Thus

$$\chi(t)=e^{-iH_0t}\chi(0), \tag{2}$$

where $\chi(0)$ must be chosen to describe the particular scattering situation envisaged, so that in particular it contains no admixture of purely bound eigenstates of the operator H_0, if any exist.

In order to prove Eq. (1), we note that $V\chi(t)=[H-i(d/dt)]\chi(t)$, so that performing an integration by parts,

$$\frac{1}{i}\int_{t_0}^{t} e^{-iH(t-\tau)}V\chi(\tau)d\tau = -\chi(t)+e^{-iHt}e^{iHt_0}e^{-iH_0t_0}\chi(0). \tag{3}$$

Now if $\chi(0)$ is a normalizable superposition of outgoing-wave basis vectors χ_a^+,

$$\chi(0)=\int c(a)\chi_a^+da, \tag{4}$$

we have[8]

$$\psi(0)\equiv\int c(a)\psi_a^+da=\lim_{t_0\to-\infty} e^{iHt_0}e^{-iH_0t_0}\chi(0). \tag{5}$$

Therefore we can take the limit as $t_0\to-\infty$ in Eq. (3), which gives Eq. (1) with $\psi(t)=e^{-iHt}\psi(0)$. It can be verified[9] that $\psi(t)$ satisfies the Schrödinger equation in the integral form

$$\psi(t)=\chi(t)+\frac{1}{i}\int_{-\infty}^{t} e^{-iH_0(t-\tau)}V\psi(\tau)d\tau. \tag{6}$$

We compute the transition amplitude $a_b(t)$ which is defined as the projection of the scattering wave function

[7] H. Ekstein, Phys. Rev. **101**, 880 (1956).

[8] M. N. Hack, Phys. Rev. **96**, 196 (1954), Eq. (15). The derivation given in this paper can be generalized to the case of modified plane waves without difficulty. The relation of ψ_a^+ to χ_a^+ is given in Eq. (20) below.

[9] Substitution of the identity

$$e^{-iH(t-\tau)}=e^{-iH_0(t-\tau)}+\frac{1}{i}\int_\tau^t e^{-iH_0(t-\tau')}Ve^{-iH(\tau'-\tau)}d\tau'$$

into Eq. (1), interchanging orders of integration with respect to τ and τ', and making use of Eq. (1) itself, leads to Eq. (6). This identity can be proved by applying the operator $i(d/dt)-H_0$ to the left- and right-hand sides. The resulting expressions are equal, so that since the identity clearly holds for $t=\tau$, it follows that it holds in general by the uniqueness theorem for solutions of differential equations.

$\psi(t)$ onto the plane-wave basis vector

$$\phi_b(t)=e^{-iKt}\phi_b=e^{-iE_bt}\phi_b, \tag{7}$$

where ϕ_b is an eigenstate of the final-state free Hamiltonian K with eigenvalue E_b. By Equations (2), (6), and (7) and in view of the self-adjointness of H_0, we have

$$a_b(t)\equiv(\phi_b(t),\psi(t))=(e^{iH_0t}e^{-iE_bt}\phi_b,\chi(0)) + \frac{1}{i}\int_{-\infty}^{t}(e^{-iH_0\tau}e^{iH_0t}e^{-iE_bt}\phi_b, V\psi(\tau))d\tau. \tag{8}$$

It can be shown (Appendix) that the limit as $t\to\infty$ of $a_b(t)$ exists and has the value which is expected by virtue of the second of the symbolic relations

$$\lim_{t\to\mp\infty} e^{iH_0t}e^{-iE_bt}\phi_b=\chi_b^{\pm}. \tag{9}$$

Here, $\chi_b^{\pm}$ are the outgoing- and ingoing-wave eigenfunctions of H_0 corresponding to ϕ_b. We thus obtain

$$a_b(\infty)=(\chi_b^-,\chi(0))-i\int_{-\infty}^{\infty}(\chi_b^-(\tau),V\psi(\tau))d\tau, \tag{10}$$

where

$$\chi_b^-(\tau)=e^{-iH_0\tau}\chi_b^-=e^{-iE_b\tau}\chi_b^-. \tag{11}$$

Letting

$$\chi(t)\to e^{-iE_at}\chi_a^+,\quad \psi(t)\to e^{-iE_at}\psi_a^+, \tag{12}$$

we get for the S matrix

$$S_{ba}=(\chi_b^-,\chi_a^+)-2\pi i\delta(E_b-E_a)(\chi_b^-,V\psi_a^+). \tag{13}$$

The ingoing-wave basis vector χ_b^- is thus seen to appear quite naturally and directly.

An alternative form of these expressions is obtained by making use of Eq. (1) and carrying out a similar calculation. The relevant symbolic relation is the second of the pair

$$\lim_{t\to\mp\infty} e^{iHt}e^{-iE_bt}\phi_b=\psi_b^{\pm}. \tag{14}$$

We obtain the alternative equivalent forms of Eqs. (10) and (13):

$$a_b(\infty)=(\chi_b^-,\chi(0))-i\int_{-\infty}^{\infty}(\psi_b^-(\tau),V\chi(\tau))d\tau, \tag{15}$$

and

$$S_{ba}=(\chi_b^-,\chi_a^+)-2\pi i\delta(E_b-E_a)(\psi_b^-,V\chi_a^+). \tag{16}$$

III. TIME-INDEPENDENT THEORY

In the present section we give the corresponding time-independent treatment for the case where the initial- and final-state basis vectors are eigenfunctions of the same unperturbed Hamiltonian H_0. In the following section we remove this restriction in order to treat rearrangement collisions on a general basis.

The outgoing- and ingoing-wave scattering eigenfunctions $\psi_b^{\pm}$ corresponding to the eigenfunctions $\chi_b^{\pm}$ of the unperturbed Hamiltonian H_0 are given by the formulas[10]

$$\psi_b^{\pm}=\chi_b^{\pm}+\frac{1}{E_b-H\pm i\epsilon}V\chi_b^{\pm}, \tag{17}$$

and satisfy the integral equations[10,11]

$$\psi_b^{\pm}=\chi_b^{\pm}+\frac{1}{E_b-H_0\pm i\epsilon}V\psi_b^{\pm}. \tag{18}$$

Here and below, the limit as ϵ approaches zero through positive values is understood. We have also the eigenvalue equations

$$H_0\chi_b^{\pm}=E_b\chi_b^{\pm},\quad \text{and}\quad H\psi_b^{\pm}=E_b\psi_b^{\pm}. \tag{19}$$

Substitution of the second of Eqs. (17) and the first of Eqs. (21),

$$\psi_a^{\pm}=\chi_a^{\pm}+\frac{1}{E_a-H\pm i\epsilon}V\chi_a^{\pm} \tag{20}$$

$$=\chi_a^{\pm}+\frac{1}{E_a-H_0\pm i\epsilon}V\psi_a^{\pm}, \tag{21}$$

into the fundamental formula[12]

$$S_{ba}=(\psi_b^-,\psi_a^+) \tag{22}$$

for the S matrix gives

$$\begin{aligned}S_{ba}&=\left(\chi_b^-+\frac{1}{E_b-H-i\epsilon}V\chi_b^-,\psi_a^+\right)\\&=(\chi_b^-,\psi_a^+)+\frac{1}{E_b-E_a+i\epsilon}(V\chi_b^-,\psi_a^+)\\&=\left(\chi_b^-,\chi_a^++\frac{1}{E_a-H_0+i\epsilon}V\psi_a^+\right)\\&\qquad+\frac{1}{E_b-E_a+i\epsilon}(\chi_b^-,V\psi_a^+)\\&=(\chi_b^-,\chi_a^+)+\left(\frac{1}{E_a-E_b+i\epsilon}+\frac{1}{E_b-E_a+i\epsilon}\right)\\&\qquad\times(\chi_b^-,V\psi_a^+),\end{aligned} \tag{23}$$

---

[10] M. Gell-Mann and M. L. Goldberger, reference 6, Eqs. (4.7)–(4.9). Equations (17) and (18) differ from the usual ones in that the modified plane-wave basis vectors $\chi_b^{\pm}$ appear instead of the plane-wave basis vector ϕ_b. However, it was recognized by Gell-Mann and Goldberger that the plane-wave basis vectors and the modified plane-wave basis vectors lead to exactly the same scattering eigenfunctions, i.e.,

$$\psi_b^{\pm}=\phi_b+\frac{1}{E_b-H\pm i\epsilon}(H-E_b)\phi_b$$

$$=\chi_b^{\pm}+\frac{1}{E_b-H\pm i\epsilon}(H-E_b)\chi_b^{\pm}.$$

[11] It may be necessary to introduce projection operators to split off purely bound states of H_0, if any exist at the energy E_b, in order that the resolvent operator be well defined. An argument similar to the one in the text can then be carried through and leads to the same result.

[12] This important formula was first given by Gell-Mann and

i.e.,

$$S_{ba}=(\chi_b^-,\chi_a^+)-2\pi i\delta(E_b-E_a)(\chi_b^-,V\psi_a^+), \quad (24)$$

which is just Eq. (13).

Similarly, by substitution of the first of Eqs. (20) and the second of Eqs. (18) into Eq. (22), we obtain Eq. (16) for the S matrix:

$$S_{ba}=(\chi_b^-,\chi_a^+)-2\pi i\delta(E_b-E_a)(\psi_b^-,V\chi_a^+). \quad (25)$$

Alternatively, the equivalence of (24) and (25) can be seen directly by taking note of the reciprocity relation

$$(\psi_b^-,V\chi_a^+)=(\chi_b^-,V\psi_a^+) \quad (\text{for } E_b=E_a). \quad (26)$$

In the case of scattering by two potentials, where the initial- and final-state free Hamiltonians are the same and $H_0=K+U$, the first term of (24) or (25) is just the expression for the S matrix as if only the potential U were acting, and we have

$$(\chi_b^-,\chi_a^+)=\delta(b-a)-2\pi i\delta(E_b-E_a)(\phi_b,U\chi_a^+). \quad (27)$$

In the case of ionization we have, by virtue of the orthogonality of the bound and continuum states of the scattering system,

$$(\chi_b^-,\chi_a^+)=0. \quad (28)$$

IV. REARRANGEMENT COLLISIONS

The difficulty encountered in treating rearrangement collisions is the fact that the initial- and final-state basis vectors are in general not eigenfunctions of the same unperturbed Hamiltonian H_0. However, an important theorem has recently been obtained which can be used to overcome this difficulty.[13] In the concise formulation due to Lippmann,[14] the theorem asserts that the outgoing- and ingoing-wave scattering eigenfunctions given by Eqs. (20) and (21) also satisfy integral equations in terms of the resolvent of the unperturbed operator H_0':

$$\psi_a^\pm=\lambda_a^{\pm\prime}+\frac{1}{E_a-H_0'\pm i\epsilon}V'\psi_a^\pm, \quad (29)$$

where

$$\lambda_a^{\pm\prime}\equiv\frac{\pm i\epsilon}{E_a-H_0'\pm i\epsilon}\chi_a^\pm, \quad (30)$$

and

$$H_0'+V'=H_0+V=H. \quad (31)$$

Here H_0 and H_0' are the initial- and final-state unperturbed Hamiltonians which differ from the initial- and final-state free Hamiltonians in the manner described in the introduction. With the help of this theorem, the treatment given in the preceding section can be extended to the present case where the initial- and final-state unperturbed Hamiltonians are no longer the same. By substitution of the second of Eqs. (32),

$$\psi_b^{\pm\prime}=\chi_b^{\pm\prime}+\frac{1}{E_b-H\pm i\epsilon}V'\chi_b^{\pm\prime}, \quad (32)$$

and the first of Eqs. (29) into the fundamental formula for the S matrix,[12]

$$S_{ba}=(\psi_b^{-\prime},\psi_a^+), \quad (33)$$

we obtain by a calculation similar to that of the preceding section the result

$$S_{ba}=(\chi_b^{-\prime},\lambda_a^{+\prime})-2\pi i\delta(E_b-E_a)(\chi_b^{-\prime},V'\psi_a^+). \quad (34)$$

An alternative form of the S matrix is obtained by making use of the first of Eqs. (20) and the second of the relations (35),

$$\psi_b^{\pm\prime}=\lambda_b^\pm+\frac{1}{E_b-H_0\pm i\epsilon}V\psi_b^{\pm\prime}, \quad (35)$$

where

$$\lambda_b^\pm\equiv\frac{\pm i\epsilon}{E_b-H_0\pm i\epsilon}\chi_b^{\pm\prime}. \quad (36)$$

Substitution into Eq. (33) gives

$$S_{ba}=(\lambda_b^-,\chi_a^+)-2\pi i\delta(E_b-E_a)(\psi_b^{-\prime},V\chi_a^+). \quad (37)$$

The equivalence of (34) and (37) can be seen directly by taking note of the relations

$$(\lambda_b^-,\chi_a^+)=(\chi_b^{-\prime},\lambda_a^{+\prime})-2\pi i\delta(E_b-E_a)(\chi_b^{-\prime},[V'-V]\chi_a^+), \quad (38)$$

and

$$(\chi_b^{-\prime},V'\psi_a^+)-(\psi_b^{-\prime},V\chi_a^+)=(\chi_b^{-\prime},[V'-V]\chi_a^+) \quad (\text{for } E_b=E_a). \quad (39)$$

With the help of Eqs. (30) and (36), it is seen that the first terms of Eqs. (34) and (37) vanish for $E_b\neq E_a$ and indeed fail to vanish for $E_b=E_a$ only if the transition amplitude $(\chi_b^{-\prime},\chi_a^+)$ between the initial- and final-state basis vectors has a singularity at $E_b=E_a$. For rearrangement collisions of the exchange type, it has been shown that there is no singularity at $E_b=E_a$,[14] so that in such cases the first terms of Eqs. (34) and (37) can be omitted.

The S matrix for rearrangement collisions can also be derived time-dependently. For this purpose the identity

$$e^{-iH_0(t-\tau)}=e^{-iH_0'(t-\tau)}+\frac{1}{i}\int_\tau^t e^{-iH_0'(t-\tau')}(H_0-H_0')\times e^{-iH_0(\tau'-\tau)}d\tau' \quad (40)$$

is useful. Substituting this identity into the integral equation (6) satisfied by $\psi(t)$, interchanging orders of

---

Goldberger, reference 6, Sec. III, Eq. (3.51). However, their derivation was not sufficiently general to encompass rearrangement collisions, and no use was made of the result. The formula was used as a basis for the time-independent theory by M. N. Hack, reference 8, and its applicability to rearrangement collisions was shown by H. Ekstein, reference 7.

[13] S. Altshuler, Phys. Rev. **91**, 1167 (1953); **92**, 1157 (1953); H. E. Moses, Phys. Rev. **91**, 185 (1953); M. Gell-Mann and M. L. Goldberger, reference 10; B. A. Lippmann, Phys. Rev. **102**, 264 (1956).

[14] B. A. Lippmann, reference 13. We have stated the theorem here in the form appropriate to modified plane waves.

integration, and making use of Eq. (6) itself and Eq. (31), we obtain the time-dependent analog of the theorem described at the beginning of this section, i.e.,

$$\psi(t)=\lambda'(t)+\frac{1}{i}\int_{-\infty}^{t} e^{-iH_0'(t-\tau)}V'\psi(\tau)d\tau, \tag{41}$$

where

$$\lambda'(t)\equiv\chi(t)+\frac{1}{i}\int_{-\infty}^{t} e^{-iH_0'(t-\tau)}(V-V')\chi(\tau)d\tau. \tag{42}$$

Making use of this result, we can derive Eq. (34) in a manner similar to that used to obtain Eq. (13). Alternatively we can make use of Eq. (1) to derive Eq. (37) as in the last paragraph of Sec. II.

Finally, we note that our results lead to an equivalence theorem[15] for the S matrix expressed in terms of modified plane waves. We obtain this theorem by carrying out two auxiliary transformations. We transform ψ_a^+ to the basis of an unperturbed Hamiltonian $\bar{H}_0$ corresponding to a different asymptotically equivalent choice of modified plane-wave basis vector for the initial state.[16] Similarly we transform $\psi_b^{-\prime}$ to the basis of an unperturbed Hamiltonian $\bar{H}_0'$ corresponding to a different equivalent choice of modified plane-wave basis vector for the final state. Here, $\bar{H}_0+\bar{V}=\bar{H}_0'+\bar{V}'=H$. We now make use of the theorem described in the beginning of this section, in the same manner as before, to derive the equations corresponding to (34) and (37):

$$\begin{aligned} S_{ba}&=(\bar{\chi}_b^{-\prime},\bar{\lambda}_a^{+\prime})-2\pi i\delta(E_b-E_a)(\bar{\chi}_b^{-\prime},\bar{V}'\psi_a^+)\\ &=(\bar{\lambda}_b^-,\bar{\chi}_a^+)-2\pi i\delta(E_b-E_a)(\psi_b^{-\prime},\bar{V}\bar{\chi}_a^+). \end{aligned} \tag{43}$$

We thus obtain a large class of alternative expressions for the S matrix by making different choices H_0, $\bar{H}_0$, H_0', $\bar{H}_0'$, etc., of unperturbed Hamiltonians corresponding to asymptotically equivalent choices of initial- and final-state basis vectors. A particular choice of basis vectors are, of course, the plane-wave basis vectors.

These results also apply to the case treated in Secs. II and III. In that case one obtains the alternative forms of the S matrix [Eqs. (24) and (25) with χ_b^-, χ_a^+, and V replaced by $\bar{\chi}_b^-$, $\bar{\chi}_a^+$, and $\bar{V}$] by making different choices of unperturbed Hamiltonians, H_0, $\bar{H}_0$, etc., corresponding to asymptotically equivalent choices of initial- and final-state basis vectors.

[15] For a related theorem, see H. Ekstein and K. Tanaka, Phys. Rev. **104**, 259 (1956).

[16] This is a transformation of the type described in reference 10. Clearly, by the relation stated there, if $\chi_a^\pm$ and $\bar{\chi}_a^\pm$ are modified plane waves corresponding to the same plane-wave basis vector ϕ_a, we have

$$\begin{aligned}\psi_a^\pm&=\chi_a^\pm+\frac{1}{E_a-H\pm i\epsilon}(H-E_a)\chi_a^\pm\\ &=\bar{\chi}_a^\pm+\frac{1}{E_a-H\pm i\epsilon}(H-E_a)\bar{\chi}_a^\pm;\end{aligned}$$

i.e., the $\psi_a^\pm$ corresponding to $\chi_a^\pm$ and $\bar{\chi}_a^\pm$ are identical.

APPENDIX

We examine the limit as $t\to\infty$ of the integral

$$I(t)=\int_{-\infty}^{t} e^{iE_bt}(\phi_b,e^{-iH_0(t-\tau)}V\psi(\tau))d\tau, \tag{44}$$

which occurs in Eq. (8). Making use of the completeness of the scattering and bound eigenstates of the self-adjoint operator H_0, we can write

$$\begin{aligned} I(t)=&\int_{-\infty}^{t}d\tau\int dc e^{iE_bt}(\phi_b,\chi_c^\pm)(\chi_c^\pm,V\psi(\tau))e^{-iE_c(t-\tau)}\\ &+\int_{-\infty}^{t}d\tau\sum_l e^{iE_bt}(\phi_b,\chi_l)(\chi_l,V\psi(\tau))e^{-iE_l(t-\tau)}. \end{aligned} \tag{45}$$

Here the $\pm$ sign denotes alternative expansions in terms of either the ingoing- or outgoing-wave scattering eigenstates, and the χ_l are the purely bound eigenstates of H_0. As will be seen, the ingoing-wave expansion is the more convenient, but both expansions lead to the same result. The scattering eigenstates of H_0 are related to those of the final-state free Hamiltonian, $K=H_0-U$, by the familiar equations

$$\begin{aligned}\chi_c^\pm&=\phi_c+\frac{1}{E_c-H_0\pm i\epsilon}U\phi_c\\ &=\phi_c+\frac{1}{E_c-K\pm i\epsilon}U\chi_c^\pm.\end{aligned} \tag{46}$$

We now make use of the well-known relations

$$\lim_{t\to\infty}\lim_{\epsilon\to0+}\left(\frac{e^{-ixt}}{x\pm i\epsilon}\right)=\begin{cases}-2\pi i\delta(x)\\ 0\end{cases}, \tag{47}$$

which are understood in the sense that the factor under the limit signs is to be multiplied by a function which is smoothly varying in the neighborhood of $x=0$ and an integration over x performed before the limits are taken. The upper and lower lines of the brace in (47) refer to the $\pm$ sign. Accordingly we have

$$\begin{aligned}\lim_{t\to\infty}&(\phi_b,\chi_c^\pm)e^{-i(E_c-E_b)t}\\ &=\lim_{t\to\infty}\lim_{\epsilon\to0+}\left(\phi_b,\phi_c+\frac{1}{E_c-E_b\pm i\epsilon}U\chi_c^\pm\right)e^{-i(E_c-E_b)t}\\ &=\begin{cases}\delta(b-c)-2\pi i\delta(E_b-E_c)(\phi_b,U\chi_c^+),\\ \delta(b-c).\end{cases}\end{aligned} \tag{48}$$

The ingoing-wave choice of the expansion therefore gives at once for the contribution of the first term in (45), in the limit as $t\to\infty$,

$$\int_{-\infty}^{\infty} e^{iE_b\tau}(\chi_b^-, V\psi(\tau))d\tau. \tag{49}$$

We next examine the contribution from the bound states χ_l. Inserting the expansion

$$\psi(\tau)=\int c(a)\psi_a{}^+e^{-iE_a\tau}da \tag{50}$$

into the second term in (45) and performing the τ integration gives in the limit $t\to\infty$ a factor

$$\int (\chi_l, V\psi_a{}^+)\delta(E_l-E_a)c(a)da. \tag{51}$$

Since χ_l is purely bound, it is permissible to make use here of the self-adjointness of H_0 between χ_l and $\psi_a{}^+$, which gives $(\chi_l, V\psi_a{}^+)=(\chi_l, [H-H_0]\psi_a{}^+)=(E_a-E_l)\times(\chi_l,\psi_a{}^+)$, so that (51) vanishes. Thus the bound states make no contribution in the limit $t\to\infty$, so that our result for $I(\infty)$ is (49), in agreement with the second term of Eq. (10).

Finally, we show that the alternative outgoing-wave choice of expansion in (45) leads to the same result. We make use of the upper line of Eq. (48) to obtain for the first term of (45) with the $+$ choice, in the limit $t\to\infty$,

$$\begin{aligned}\int_{-\infty}^{\infty} & e^{iE_b\tau}(\chi_b^+, V\psi(\tau))d\tau+\int_{-\infty}^{\infty}d\tau\int dce^{iE_b\tau} \\ & \times(2\pi i\delta(E_b-E_c)\phi_b, U\chi_c{}^+)(\chi_c{}^+, V\psi(\tau)) \\ &=\int_{-\infty}^{\infty} e^{iE_b\tau}(\chi_b^+, V\psi(\tau))d\tau+\int_{-\infty}^{\infty}d\tau\int dce^{iE_b\tau} \\ & \times(2\pi i\delta(E_b-H_0)U\phi_b,\chi_c{}^+)(\chi_c{}^+, V\psi(\tau)).\end{aligned} \tag{52}$$

We may add a term with $\int dc\cdots$ replaced by $\sum_l\cdots$ and $\chi_c{}^+$ replaced by χ_l since this term is equal to zero. Making use of the completeness, we therefore obtain

$$\begin{aligned}\int_{-\infty}^{\infty} & e^{iE_b\tau}(\chi_b^+, V\psi(\tau))d\tau+\int_{-\infty}^{\infty} e^{iE_b\tau} \\ & \times(2\pi i\delta(E_b-H_0)U\phi_b, V\psi(\tau))d\tau \\ &=\int_{-\infty}^{\infty} e^{iE_b\tau}(\chi_b^-, V\psi(\tau))d\tau,\end{aligned} \tag{53}$$

since, by (46),

$$\chi_b^- - \chi_b^+ = 2\pi i\delta(E_b-H_0)U\phi_b. \tag{54}$$

The result (53) is seen to be in agreement with (49).

We have in the above derivation for simplicity not distinguished between the various types of scattering states, but a separate treatment of the contributions from the purely continuum and the mixed partly-bound, partly-continuum scattering states leads to the same result.

The first term of Eq. (10) can be derived in a similar manner.