Boundary Conditions and Time-Dependent States

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In a previous paper, a phenomenological description of nuclear reactions by means of boundary conditions was introduced. These boundary conditions that connect the several stages of the reaction (initial particles, compound nucleus, etc.) apply to time-dependent, as well as to stationary states. It is possible to discuss then the time development of any state specified initially. In the present paper a time-dependent description is obtained for the single-level S-wave scattering of two spinless particles, and for the process of disintegration of a compound particle. The only parameters on which this time-dependent description depends are the poles of the scattering matrix. The connection between the position of the poles of the scattering matrix in the complex plane, and the time-dependent behavior of the scattering and disintegration processes, is discussed. The form of the transient scattered current is also obtained. The generalized Hankel transforms on which the present developments are based, will be shown in a following paper to be a consequence of the expansion theorems for states in Fock space.

I. INTRODUCTION

IN a previous article[1] a phenomenological description of nuclear reactions was introduced, in which the several stages of the nuclear reaction were described in an appropriate Fock space.[2] It was shown there that the boundary conditions imposed on the components of the Fock wave function lead, for stationary states, to the same dependence of the cross sections on energy as would be obtained from any of the usual formulations of resonance reaction theory.[3]

An advantage of this description is that the boundary conditions obtained hold for time dependent states, as well as for stationary states. We can then deal, not only with such problems as the dependence of the cross sections on energy, which are of an essentially stationary nature, but also with problems such as the time development of a state specified at a given initial time.

We propose to discuss in this paper, the description in time of a scattering process, and the process of disintegration of a compound particle. We shall show the dependence of this description on the position of the poles of the scattering matrix.[4] The present developments will have then, a bearing on the connection of causality with the position of the poles of the scattering matrix, recently discussed by Schützer and Tiomno.[5]

With the help of the time-dependent state for a scattering process, we will also obtain the transient scattered current that appears before stationary conditions are established.

Our aim in the present paper is to obtain a set of basic time-dependent wave functions, with the help of which we shall discuss, in a following publication, the description of interactions through boundary conditions in Fock space, from a general quantum-mechanical standpoint. We shall show there that a time dependent matrix $\mathbf{U}(t)$ can be introduced, which provides all the information concerning our states and the observables associated with them that is of relevance in quantum mechanics. The interactions through boundary conditions in Fock space will be seen then to give as complete a description of the interaction process between particles as could be obtained if they interacted through a potential.

While the present discussion is nonrelativistic, it is hoped that the restriction of the interactions to the point of coincidence[1] of the colliding particles, will permit a comparatively simple extension to the relativistic range.

In the previous note, boundary conditions were obtained for several types of scattering and reaction problems, but in order to keep mathematical complications to a minimum, we shall restrict the discussion in this, and the following paper, to the interactions between two spinless particles leading to single-level S-wave scattering. The extension to other, more complex, types of interactions will be presented in a later publication.

According to what was said in the previous note, the state representing a single-level scattering process could be found in two stages. In the first stage, two particles of masses m_1, m_2 are present, while in the second, there is only a single compound particle of mass M. If we choose the center-of-mass frame of reference, the first stage is represented by the wave function $\psi_1(\mathbf{r}, t)$ where $\mathbf{r}$ is the relative position vector of the two particles, while the second stage is represented by the wave function $\psi_2(t)$. The Fock wave function for the state is then

$$\Psi(t)=\begin{bmatrix}\psi_1(\mathbf{r}, t)\\ \psi_2(t)\end{bmatrix}. \quad (1)$$

[1] M. Moshinsky, Phys. Rev. **81**, 347 (1951). This paper will be referred to as "previous note."
[2] V. Fock, Z. Physik **75**, 622 (1932).
[3] E. P. Wigner and L. Eisenbud, Phys. Rev. **72**, 29 (1947); G. Breit, Phys. Rev. **69**, 472 (1946); Feshbach, Peaslee, and Weisskopf, Phys. Rev. **71**, 145 (1947).
[4] J. A. Wheeler, Phys. Rev. **52**, 1107 (1937); W. Heisenberg, Z. Physik **120**, 513, 673 (1943); E. P. Wigner, Phys. Rev. **70**, 15 (1946).
[5] W. Schützer and J. Tiomno, Phys. Rev. **83**, 249 (1951). I am indebted to Drs. Schützer and Tiomno for a copy of their paper prior to publication.

To simplify the notation,[6] we now choose our units so that $\hbar=1$, $c=1$ and the reduced mass

$$\mu=(m_1m_2)(m_1+m_2)^{-1}=1.$$

We have from the previous note, that for $\mathbf{r}\neq 0$, $\psi_1(\mathbf{r}, t)$ satisfies the free particle Schrödinger equation:

$$-i(\partial\psi_1/\partial t)=\tfrac{1}{2}\nabla^2\psi_1 \tag{2}$$

and that the boundary conditions that determine the interaction are:[7]

$$-i(\partial\psi_2/\partial t)+E_0\psi_2=2\pi C'(\partial r\psi_1/\partial r)_{r=0}, \tag{3}$$

$$C'\psi_2=(r\psi_1)_{r=0}. \tag{4}$$

In (3), $E_0=[M-(m_1+m_2)]$ stands for the binding energy of the compound particle, and C' is a coupling constant whose physical significance will be given below.

We could eliminate ψ_2 between (3) and (4) and obtain a boundary condition in terms of ψ_1 alone, having the form:

$$-i(\partial r\psi_1/\partial t)_{r=0}+E_0(r\psi_1)_{r=0}=2\pi C'^2(\partial r\psi_1/\partial r)_{r=0}. \tag{5}$$

For a stationary wave function

$$\psi_1(\mathbf{r}, t)=\psi(\mathbf{r})\exp(-iE''t)$$

the boundary condition reduces to the familiar form:[8]

$$(r\psi)_{r=0}=C^2(k_0^2-k''^2)^{-1}(\partial r\psi/\partial r)_{r=0}, \tag{6}$$

where[9] $C=(4\pi)^{\frac{1}{2}}|C'|$, $E''=\frac{1}{2}k''^2$, $E_0=\frac{1}{2}k_0^2$. This condition determines completely the scattering problem, as the stationary ψ must be given by a plane plus a scattered wave, and the scattered wave must be an S-wave since otherwise $r\psi$ would be singular at $r=0$. The coefficent of the scattered wave is determined by (6) and so $\psi(\mathbf{r})$ takes the form:

$$\psi(\mathbf{r})=\exp(i\mathbf{k}''\cdot\mathbf{r})+C^2(k_0^2-k''^2-ik''C^2)^{-1}r^{-1}\exp(ikr). \tag{7}$$

The total cross section is then given by the usual single level formula:

$$\sigma=(4\pi/k''^2)\Gamma^2[(E_0-E'')^2+\Gamma^2]^{-1}, \tag{8}$$

where $\Gamma=\Gamma_0(k''/k_0)$ and $\Gamma_0=\frac{1}{2}C^2k_0$. This correlates the magnitude of the coupling constant C' with the width of the energy level at resonance Γ_0 and, as will be shown later, with the probability of decay of the compound system.

At first sight, one would be inclined to think that the generalization of the boundary condition (6) for stationary states, to time-dependent states, could be achieved in terms of a single wave function $\psi_1(\mathbf{r}, t)$ satisfying (2) and (5). The discussion of the many-level scattering process in the previous note, as well as the form of similar vibration problems,[10] show though, that the generalization should be made in terms of the formulation (1)–(4) in Fock space.

Having now the information concerning stationary states that our interactions through boundary conditions can provide, we want to investigate the behavior of time-dependent states. We shall discuss, in the present paper, two time-dependent states. The first one will be the state which initially is found in the form of two particles with relative momentum $\mathbf{k}''$, so that its development in time will provide a causal description of a resonance scattering process. The second, will be a state which initially is found in the form of a single compound particle, so that its development in time will provide a causal description of a disintegration process. The Fock wave functions corresponding to these two states, will be designated by Ψ_1, Ψ_2, where:

$$\Psi_1(\mathbf{k}'', t)=\begin{bmatrix}\psi_{11}(\mathbf{r}, \mathbf{k}'', t)\\ \psi_{21}(\mathbf{k}'', t)\end{bmatrix}, \quad \Psi_2(t)=\begin{bmatrix}\psi_{12}(\mathbf{r}, t)\\ \psi_{22}(t)\end{bmatrix}, \tag{9a, b}$$

and according to what was said above, we have that for $t=0$:

$$\Psi_1(\mathbf{k}'', 0)=(2\pi)^{-\frac{3}{2}}\begin{bmatrix}\exp(i\mathbf{k}''\cdot\mathbf{r})\\ 0\end{bmatrix}, \quad \Psi_2(0)=\begin{bmatrix}0\\ 1\end{bmatrix}. \tag{10a, b}$$

We will show in what follows, that the Eq. (2) and the boundary conditions (3, 4), satisfied by the components of the time-dependent Fock wave functions, determine these wave functions completely, once the initial form of them is given. In the next section, we will discuss a mathematical preliminary which is necessary for this determination.

II. GENERALIZED HANKEL TRANSFORMS

Any wave function $\psi_1(\mathbf{r}, t)$ representing that stage of our state in which two particles are present, can be developed in spherical waves according to well known rules.[11] As the boundary conditions (3, 4) allow only S-wave scattering, it is clear that we can restrict our discussion of time-dependent wave functions to the first term in the spherical wave development, i.e., to $l=0$. The terms in the development of $\psi_1(\mathbf{r}, t)$ corresponding to relative angular momentum higher than 0, will behave as free particle wave functions.

[6] The units for time, length, and mass are then $\hbar(\mu c^2)^{-1}$, $\hbar(\mu c)^{-1}$, and μ, respectively. All quantities that appear in the following developments are therefore dimensionless.

[7] In this article we consider that $i\partial/\partial t$ is the operator for the kinetic energy alone, i.e., we have eliminated a phase factor $\exp[-i(m_1+m_2)t]$ from the formulation of the previous note. The coupling constant C_{12} of the previous note will be assumed real and denoted by C', while C_{11} will be taken as zero, so that there is no direct coupling between the two particles in the first stage.

[8] E. P. Wigner, Phys. Rev. **73**, 1002 (1948).

[9] We shall designate by E'' the relative kinetic energy, and by $\mathbf{k}''$ the corresponding momentum of the two particles, as this would be appropriate in the bra and ket notation, to be introduced in the following article.

[10] A. G. Webster, *Partial Differential Equations in Mathematical Physics* (G. E. Stechert & Company, New York, 1933), second edition, pp. 124–129.

[11] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon Press, Oxford, 1949), second edition, p. 22.

Before we attempt to obtain the explicit form of the time-dependent Fock states, let us look at the well-known procedure one follows in the case of two non-interacting particles. Let us assume that in the center-of-mass reference frame, we have two noninteracting particles with zero relative angular momentum, represented at $t=0$ by the wave packet $\psi(r)$. The Hankel transform corresponding to this wave packet is:

$$F(k)=(2/\pi)^{\frac{1}{2}}\int_0^\infty \psi(\rho)(k\rho)^{-1}\sin k\rho\ \rho^2 d\rho, \quad (11a)$$

$$\psi(r)=(2/\pi)^{\frac{1}{2}}\int_0^\infty F(k)(kr)^{-1}\sin kr\ k^2 dk. \quad (11b)$$

With the help of (11), the time dependent wave function can then be explicitly obtained in the form:

$$\psi(r,t)=(2/\pi)^{\frac{1}{2}}\int_0^\infty F(k)(kr)^{-1}\sin kr\exp(-i\tfrac{1}{2}k^2t)k^2dk. \quad (12)$$

The relations (11) are, of course, connected with the expressions in transformation theory, that take us from the configuration to the energy-angular momentum representation of the state. The transform $F(k)$ can also be expressed as an integral over all of configuration space, in the form:

$$F(k)=(2\pi)^{-\frac{3}{2}}\int (kr)^{-1}\sin kr\ \psi(r)\ d\mathbf{r}, \quad (11c)$$

i.e., as $(2\pi)^{-\frac{3}{2}}$ times the scalar product of the two wave functions in the integrand.

From the above, we see that the explicit form for time-dependent Fock states could be found, if we had an appropriate generalization of the Hankel transforms (11). For this, we introduce a stationary Fock wave function corresponding to zero relative angular momentum for the two particles of the form:

$$\Phi(k)=\begin{bmatrix}\phi_1(k,r)\\ \phi_2(k)\end{bmatrix}. \quad (13)$$

The component $\phi_1(k,r)$ of (13) is defined so as to satisfy $\nabla^2\phi_1+k^2\phi_1=0$ and the boundary condition (6), and to reduce in the absence of interaction (i.e., $C=0$) to $(kr)^{-1}\sin kr$. For $\phi_1(k,r)$ we have then:

$$\phi_1(k,r)=(-2ikr)^{-1}[\exp(-ikr)-S(k)\exp(ikr)] \quad (14)$$

where $S(k)$, the single component of the scattering matrix,[4] is determined by the boundary condition (6), so that it becomes:

$$S(k)=(k_0^2-k^2-ikC^2)^{-1}(k_0^2-k^2+ikC^2). \quad (15)$$

The component $\phi_2(k)$ of (13) is determined by the boundary condition (4), so that $\Phi(k)$ takes finally the form:

$$\Phi(k)=\begin{bmatrix}\dfrac{kC^2}{k_0^2-k^2-ikC^2}\left(\dfrac{\cos kr}{kr}+\dfrac{k_0^2-k^2}{kC^2}\dfrac{\sin kr}{kr}\right)\\ 4\pi C'(k_0^2-k^2-ikC^2)^{-1}.\end{bmatrix}. \quad (16)$$

Let us now designate by Ψ any other Fock state in which in the first stage, the two particles have zero relative angular momentum, so that at $t=0$, Ψ has the form:

$$\Psi=\begin{bmatrix}\psi_1(r)\\ \psi_2\end{bmatrix}. \quad (17)$$

The scalar product (Φ,Ψ) of the two Fock states is, according to the previous note, given by:

$$(\Phi,\Psi)=\int \phi_1^*\psi_1 d\mathbf{r}+\phi_2^*\psi_2. \quad (18)$$

We can now give a formal generalization of the Hankel transforms (11), in terms of the relations:

$$F(k)=(2\pi)^{-\frac{3}{2}}(\Phi,\Psi)=(2/\pi)^{\frac{1}{2}}\int_0^\infty \phi_1^*(k,\rho)\psi_1(\rho)\rho^2 d\rho + (2\pi)^{-\frac{3}{2}}\phi_2^*(k)\psi_2, \quad (19a)$$

$$\Psi=\begin{bmatrix}\psi_1(r)\\ \psi_2\end{bmatrix}=(2/\pi)^{\frac{1}{2}}\int_0^\infty F(k)\begin{bmatrix}\phi_1(k,r)\\ \phi_2(k)\end{bmatrix}k^2dk. \quad (19b)$$

In the absence of interactions, i.e., when $C=0$ the relation (19) reduces to (11). A justification of the relation (19) from a quantum-mechanical standpoint, will be given in a following paper in which the $\Phi(k)$'s are shown to be the eigen Fock states of a complete set of commutaing observables, including an appropriately defined hamiltonian, as well as the relative angular momentum operator. The relation (19) indicates that a Fock state Ψ corresponding to the same relative angular momentum eigenvalue $l=0$ than $\Phi(k)$ does, can be expanded[12] in terms of the basic eigenstates $\Phi(k)$ corresponding to eigenvalues $E=\frac{1}{2}k^2$ of the hamiltonian. A rigorous mathematical derivation of (19) can also be given with the help of the functional methods developed by Kneser,[13] Hilb and others, and it will be presented elsewhere.

With the help of (19), we obtain the explicit form of the time dependent Fock state $\Psi(t)$ corresponding to the initial value (17), which is given by:

$$\Psi(t)\equiv\begin{bmatrix}\psi_1(r,t)\\ \psi_2(t)\end{bmatrix}=(2/\pi)^{\frac{1}{2}}\int_0^\infty F(k)\begin{bmatrix}\phi_1(k,r)\\ \phi_2(k)\end{bmatrix} \times\exp(-i\tfrac{1}{2}k^2t)k^2dk, \quad (20)$$

where $F(k)$ is defined by (19a).

[12] P. A. M. Dirac, *Quantum Mechanics* (Clarendon Press, Oxford, 1947), third edition, Chap. III, p. 64.

[13] A. Kneser, *Die Integralgleichungen und ihre Anwendung in der mathematischen Physik* (Vieweg, Braunschweig, Germany, 1922), second edition, Chapter VI, p. 236.

From (20) we see that the components of $\Psi(t)$ satisfy the boundary condition (4), as $[r\phi_1(k,r)]_{r=0}=C'\phi_2(k)$ from definition. Furthermore, we see from the form (16) of $\Phi(k)$, that the components of $\Psi(t)$ will satisfy the Schrödinger equation (2) and the boundary condition (3), in case we can interchange the differentiation procedures involved with the integral sign in (20).

III. TIME DEPENDENT STATES FOR SCATTERING AND DISINTEGRATION

We shall first determine the time-dependent state $\Psi_1(\mathbf{k}'',t)$ which gives a causal description of the resonance scattering process. Its initial form is given by (10a), which may be written as:

$$(2\pi)^{\frac{3}{2}}\Psi_1(\mathbf{k}'',0)=\begin{bmatrix}(k''r)^{-1}\sin k''r\\0\end{bmatrix}+\begin{bmatrix}\exp(i\mathbf{k}''\cdot\mathbf{r})-(k''r)^{-1}\sin k''r\\0\end{bmatrix}. \quad (21)$$

The second summand, when expanded in spherical waves,[11] represents a superposition of states for which the relative angular momentum $l>0$. According to the remarks of the previous section, we see that the second summand represents a noninteracting system of two particles, and the corresponding time-dependent behavior is obtained by multiplication with $\exp(-iE''t)$.

The time-dependent state represented initially by the first summand of (21), can be obtained with the help of (19a, 20), and if we designate the first component of this time-dependent state by $\psi_1(r,k'',t)$, we can write:

$$(2\pi)^{\frac{3}{2}}\psi_{11}(\mathbf{r},\mathbf{k}'',t)=[\psi_1(r,k'',t)-(k''r)^{-1}\sin(k''r)\exp(-i\tfrac{1}{2}k''^2t)]+\exp i[\mathbf{k}''\cdot\mathbf{r}-\tfrac{1}{2}k''^2t], \quad (22a)$$

$$(2\pi)^{\frac{3}{2}}\psi_{21}(\mathbf{k}'',t)=(1/C')[r\psi_1(r,k'',t)]_{r=0}. \quad (22b)$$

The last relation coming from the first, when we apply the boundary condition (4).

The time dependent state $\Psi_1(\mathbf{k}'',t)$ is completely determined once $\psi_1(r,k'',t)$ is known, and this, in turn, is given by (19, 20) of the previous section, if we introduce there, for the initial state, the form $\psi_1(r)=(k''r)^{-1}\sin k''r$, $\psi_2=0$. The calculations are carried in Appendix 1, and with the help of the results obtained there, we can write the first component of $\Psi_1(\mathbf{k}'',t)$ in the form:

$$(2\pi)^{\frac{3}{2}}\psi_{11}(\mathbf{r},\mathbf{k}'',t)=\exp i[\mathbf{k}''\cdot\mathbf{r}-\tfrac{1}{2}k''^2t]-\frac{C^2}{r}\left\{\frac{k_1\chi(r,k_1,t)}{(k_1^2-k''^2)(k_1-k_2)}+\frac{k_2\chi(r,k_2,t)}{(k_2^2-k''^2)(k_2-k_1)}-\frac{\chi(r,k'',t)}{2(k_0^2-k''^2-ik''C^2)}-\frac{\chi(r,-k'',t)}{2(k_0^2-k''^2+ik''C^2)}\right\}, \quad (23)$$

where for any complex k, we have:

$$\chi(r,k,t)=\exp i(kr-\tfrac{1}{2}k^2t)\times\operatorname{erfc}[(1-i)(4t)^{-\frac{1}{2}}(r-kt)], \quad (24)$$

and erfc(z) stands for the error integral function defined by:[14]

$$\operatorname{erfc}(z)=2\pi^{-\frac{1}{2}}\int_z^\infty\exp(-z^2)dz=1-\operatorname{erf}(z). \quad (25)$$

The only parameters that appear in the wave function (23) are k_1, k_2, which correspond to the values of k at the poles of the scattering matrix (15). Accordingly, k_1, k_2 are the roots of the equation:

$$k_0^2-k^2-ikC^2=0 \quad (26a)$$

and so, take the values:

$$\left.\begin{matrix}k_1\\k_2\end{matrix}\right\}=k_0\{\pm[1-(C^2/2k_0)^2]^{\frac{1}{2}}-i(C^2/2k_0)\}. \quad (26b)$$

The second component of $\Psi_1(\mathbf{k}'',t)$ can be obtained from (23) with the help of the boundary condition (4), so that we have:

$$(2\pi)^{\frac{3}{2}}\psi_{21}(\mathbf{k}'',t)=-4\pi C'\{\ \}_{r=0}, \quad (23a)$$

where the terms in the bracket are those inside the curly bracket of (23) evaluated at $r=0$.

The time-dependent state $\Psi_2(t)$, which gives a causal description of the disintegration process, is given initially by (10b), so its explicit form can be obtained from (19, 20) if we put there $\psi_1(r)=0$, $\psi_2=1$. For the calculations we again refer to Appendix 1, and we have, for the first component of $\Psi_2(t)$ the form:

$$\psi_{12}(\mathbf{r},t)=C'r^{-1}(k_1-k_2)^{-1}[k_1\chi(r,k_1,t)-k_2\chi(r,k_2,t)]. \quad (27a)$$

For the second component of $\Psi_2(t)$ we use the boundary condition (4), and we have:

$$\psi_{22}(t)=(k_1-k_2)^{-1}[k_1\chi(0,k_1,t)-k_2\chi(0,k_2,t)]. \quad (27b)$$

We have obtained in this section the explicit form of the time-dependent states $\Psi_1(\mathbf{k}'',t)$, $\Psi_2(t)$, representing the causal description of the process of resonance elastic scattering, and disintegration, respectively. In the following section, we will show that the components of these states satisfy Eq. (2) and the boundary conditions (3), (4), as well as the initial conditions (10a, b). We shall also discuss the asymptotic behavior of these time-dependent states when $t\to\infty$, as well as its dependence on the position of the poles of the scattering matrix, which are the only parameters present.

[14] E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, New York, 1943), American edition, pp. 341–343.

IV. PROPERTIES OF THE TIME-DEPENDENT STATES

Using the definition (24) of $\chi(r, k, t)$ we can easily check by direct substitution that:

$$\tfrac{1}{2}(\partial^2\chi/\partial r^2) = -i(\partial\chi/\partial t). \tag{28a}$$

It is clear therefore, that $r^{-1}\chi(r, k, t)$ satisfies Eq. (2) for any complex k. We see from the forms (23) (27a) of the first components of $\Psi_1(\mathbf{k}'', t)$, $\Psi_2(t)$, that they satisfy the time dependent Schrödinger equation (2) for $\mathbf{r}\neq 0$.

The components of $\Psi_1(\mathbf{k}'', t)$, $\Psi_2(t)$ must satisfy the boundary conditions (3, 4), and since (4) is always valid, as seen in (20), we can reduce the boundary condition (3) to the form (5) in which only the first component of the Fock state appears. Again, we need a property of the $\chi(r, k, t)$ which from its definition (24), is seen to satisfy the relation:

$$-i(\partial\chi/\partial t)_{r=0} + \tfrac{1}{2}k_0^2(\chi)_{r=0} - \tfrac{1}{2}C^2(\partial\chi/\partial r)_{r=0}$$
$$= \tfrac{1}{2}(k_0^2 - k^2 - ikC^2)(\chi)_{r=0} + (4\pi t)^{-\frac{1}{2}}(1-i)(C^2-ik). \tag{28b}$$

Making use of (28b), which is valid for any complex k, and of the fact that k_1, k_2 are the roots of Eq. (26a), we can prove by direct substitution that $\psi_{11}(\mathbf{r}, \mathbf{k}'', t)$ and $\psi_{12}(\mathbf{r}, t)$ satisfy (5).

Finally, we want to show that $\Psi_1(\mathbf{k}'', t)$, $\Psi_2(t)$ reduce at $t=0$ to the initial values (10a, b). This is achieved with the help of the properties of $\chi(r, k, t)$. First, if $r\neq 0$ and $t\to 0$, $\chi(r, k, t)\to 0$, because the factor,

$$\operatorname{erfc}[(1-i)(4t)^{-\frac{1}{2}}(r-kt)]\to\operatorname{erfc}[(1-i)\infty]\to 0,$$

as seen in Appendix 2. From this we see immediately that for $t\to 0$, $\psi_{11}(\mathbf{r}, \mathbf{k}'', t)\to(2\pi)^{-\frac{3}{2}}\exp i\mathbf{k}''\cdot\mathbf{r}$ and $\psi_{12}(\mathbf{r}, t)\to 0$. Now, if $r=0$, then

$$\chi(0, k, t) = \exp(-i\tfrac{1}{2}k^2t)\operatorname{erfc}[-(1-i)k(t/4)^{\frac{1}{2}}],$$

which from the definition (25) of erfc(z) takes for $t=0$ the value $\chi(0, k, 0)=1$. Accordingly, $\psi_{21}(\mathbf{k}'', t)$ reduces to the sum of the coefficients of the χ's contained in the curly bracket of (23), which is seen to be zero, so that $\psi_{21}(\mathbf{k}'', 0)=0$. From (27b) we see also that $\psi_{22}(0)=1$, so that the initial conditions (10a, b) hold.

The above analysis is seen to be independent of the position of k_1, k_2 in the complex k-plane, so long as k_1, k_2 are roots of Eq. (26a).

V. ASYMPTOTIC BEHAVIOR

We are interested now in the asymptotic form of our time-dependent states $\Psi_1(\mathbf{k}'', t)$, $\Psi_2(t)$ when $t\to\infty$, as this form should be the one corresponding to stationary states for scattering and disintegration, respectively. As the only parameters that appear in the explicit expressions of these states, are the poles of the scattering matrix, we see that these asymptotic forms will depend on the position of k_1, k_2 in the complex k-plane.

As k_1, k_2 are roots of (26a), we see that their values depend on those of the binding energy $E_0=\frac{1}{2}k_0^2$ and the coupling constant C^2. From the previous note, we see that C^2 must be real and positive if conservation of probability holds. The binding energy E_0 must be real, but it can be positive or negative. We see from (26b) that if $C^2>0$, $E_0>0$ and $(C^2/2k_0)<1$, then k_1, k_2 are in the lower half of the complex k-plane symmetrically situated with respect to the imaginary axis. If $(C^2/2k_0)\geqslant 1$ then they are both on the negative imaginary axis. In case $E_0<0$, *i.e.*, $k_0=i\kappa_0$ where κ_0 is real >0, then k_1 is on the upper and k_2 on the lower imaginary axis. For any physically significant case, the poles of the scattering matrix are then, either in the lower half of the k-plane, or on the imaginary axis, and the general character of this result has been shown by Schützer and Tiomno.[5] We shall also investigate the possibility that the poles of the scattering matrix are on the upper half of the k-plane, to see how the causal description is affected.

To obtain the asymptotic behavior of our states, we need to know the asymptotic form of $\chi(r, k, t)$ for a given r and complex k, when $t\to\infty$. In Appendix 2 we show that when $t\to\infty$ we have:

$$\chi(r, k, t)\to 2\exp[i(kr-\tfrac{1}{2}k^2t)] \text{ when } -\tfrac{1}{4}\pi<\arg k<\tfrac{3}{4}\pi, \tag{29a}$$

$$\chi(r, k, t)\to 0, \text{ when } \tfrac{3}{4}\pi<\arg k<(7\pi/4). \tag{29b}$$

These relations hold also for $r=0$.

(a) Binding Energy $E_0>0$

We saw that in this case k_1, k_2 are in the lower half of the k-plane. Now we consider two separate possibilities, (i) $-\frac{1}{4}\pi\leqslant\arg k_1\leqslant 0$, (ii) $-\frac{1}{2}\pi\leqslant\arg k_1<-\frac{1}{4}\pi$. In the second case (ii), we have that $-k''$, k_2, k_1 are in the range indicated in (29b) so that the corresponding χ's$\to 0$, and in (23) we are left only with $\chi(r, k'', t)$, whose asymptotic form is given by (29a), so that finally:

$$(2\pi)^{\frac{3}{2}}\psi_{11}(\mathbf{r}, \mathbf{k}'', t)\to\left[\exp i\mathbf{k}''\cdot\mathbf{r} + \frac{C^2}{k_0^2 - k''^2 - ik''C^2}\times\frac{\exp ik''r}{r}\right]\exp(-i\tfrac{1}{2}k''^2t). \tag{30a}$$

The same result is obtained in the first case (i) because though $\chi(r, k_1, t)$ has then the asymptotic form (29a), the imaginary part of k_1^2 is negative and $\exp(-i\frac{1}{2}k_1^2t)\to 0$ when $t\to\infty$.

For binding energy $E_0>0$, the Fock state $\Psi_1(\mathbf{k}'', t)$ tends asymptotically to the stationary state (7) corresponding to the resonance scattering process.

It is of interest to consider the asymptotic form of the Fock state for disintegration $\Psi_2(t)$, in the physically important case, when the width of energy levels at resonance is much smaller than the separation of the levels, which in this case means $(\Gamma_0/E_0)\ll 1$. From (8) we have that $(C^2/k_0)=(\Gamma_0/E_0)\ll 1$, and from (26b) we see that case (i) holds. From the expression (27b) for $\psi_{22}(t)$ we see that its asymptotic form is:

$$2k_1(k_1-k_2)^{-1}\exp(-i\tfrac{1}{2}k_1^2t). \tag{30b}$$

According to the interpretation given to the components of a Fock state in the previous note, we see that $\psi_{22}^*(t)\psi_{22}(t)$ represents the probability of observing a state originally in the form of a single particle, still in that form at time t. From (30b), and the fact that $k_1^2 \simeq k_0^2 - iC^2k_0$, we see that this probability is given by:

$$\text{const}\exp(-C^2k_0t) \tag{30c}$$

and so, the width $\Gamma_0=\frac{1}{2}C^2k_0$ is related with the probability of disintegration of the compound particle, as one should expect.[15]

(b) Binding Energy $E_0<0$

In this case, k_1 is on the upper and k_2 on the lower imaginary axis, and therefore, $-k''$, k_2 have their arguments in the range (29b), so that the corresponding χ's$\to 0$, while the χ's corresponding to k'', k_1 have the asymptotic form (29a). It is clear then, that the asymptotic form of $(2\pi)^{\frac{1}{2}}\psi_{11}(\mathbf{r}, \mathbf{k}'', t)$ is given by (30a) plus the term:

$$2C^2\kappa_1(\kappa_1^2+k''^2)^{-1}(\kappa_1+\kappa_2)^{-1} \times[r^{-1}\exp(-\kappa_1 r)\exp(i\tfrac{1}{2}\kappa_1^2 t)], \tag{31}$$

where $k_1=i\kappa_1$, $k_2=-i\kappa_2$, and κ_1, κ_2 real >0.

The term in the square bracket of (31) is seen to satisfy Eq. (2) and the boundary condition (5), and it goes exponentially to zero when $r\to\infty$. It represents then a bound state corresponding to the negative energy $E_1=-\frac{1}{2}\kappa_1^2$, and its appearance in the stationary state for scattering just tells us that for $E_0<0$, i.e., $M<(m_1+m_2)$, a stable bound state can be formed as a result of the collision. Because of its behavior when $r\to\infty$ this bound state does not change the dependence of the cross section on energy, which continues to be given by (8).

From (27a) we see that when $t\to\infty$, $\psi_{12}(\mathbf{r}, t)$ tends, except for a constant factor, to the form (31). The Fock state $\Psi_2(t)$ tends then asymptotically to the above bound state of negative energy E_1.

(c) Poles of the Scattering Matrix in the Upper Half-Plane

As the poles of the scattering matrix k_1, k_2 are roots of Eq. (26a), they can be in the upper half-plane (excluding the imaginary axis), only if we abandon the restriction that C^2, E_0 are real and that $C^2>0$. We cannot though give arbitrary complex values to E_0, C^2 as the fundamental properties[16] of the S-matrix for real k:

$$S(k)S(-k)=1, \quad S^*(k)S(k)=1$$

must be preserved. To satisfy this restriction, we see that E_0, C^2 in (15) must remain real and we have only the freedom of taking $C^2<0$. In this case the poles k_1, k_2 when outside the imaginary axis, will be situated in the upper half-plane symmetrically with respect to this axis.

[15] E. Fermi, *Nuclear Physics* (University of Chicago Press, Chicago, 1950), revised edition, p. 154.
[16] Ning Hu, Phys. Rev. **74**, 132 (1948).

We indicate by k_1 the pole in the first quadrant, and by k_2 the pole in the second. Now, if $(3\pi/4)<\arg k_2<\pi$ the corresponding χ goes to zero, while in case $(\pi/2)<\arg k_2\leqslant(3\pi/4)$ the χ has the asymptotic form (29a) but this, in turn, goes to zero when $t\to\infty$ because k_2^2 has a negative imaginary part. We need to concern ourselves only with the χ's in (23) corresponding to k'', k_1. The asymptotic form for $\chi(r, k_1, t)$ is given by (29a), *and it goes to* ∞ when $t\to\infty$ because the imaginary part of k_1^2 is positive. The wave function $\psi_{11}(\mathbf{r}, \mathbf{k}'', t)$ will go then to ∞ when $t\to\infty$.

For poles in the upper half-plane (excluding the imaginary axis), it is not possible to give a causal description of the scattering process in terms of a wave function $\psi_{11}(\mathbf{r}, \mathbf{k}'', t)$, connecting the initial plane wave with a final plane plus scattered waves. This is in line with the general results of Schützer and Tiomno.[5]

VI. THE TRANSIENT SCATTERED CURRENT

In a scattering process, our main interest lies in the determination of the scattered current, which is directly connected with the cross section. As in the present analysis we have obtained a time dependent state $\psi_{11}(\mathbf{r}, \mathbf{k}'', t)$ for the description of the scattering process, we see that we are in a position to determine, not only the stationary scattered current that is established when $t\to\infty$, but also the transient scattered current that appears between the initiation of the phenomenon and the establishment of stationary conditions.

From (23) we see that $(2\pi)^{\frac{1}{2}}\psi_{11}(\mathbf{r}, \mathbf{k}'', t)$ is given by a plane plus a scattered S-wave, which we shall designate by $\psi_S(r, k'', t)$, and whose form is:

$$\psi_S(r, k'', t)=-C^2r^{-1}\sum_{i=1}^{4}A_i\chi(r, k_i, t), \tag{32}$$

where k_1, k_2 are, as before, the poles of the scattering matrix, $k_3=k''$, $k_4=-k''$ and the A_i's are the coefficients of the corresponding χ's in (23).

The scattered current $\mathbf{j}$ is expressed in the usual form in terms of the ψ_S, and the flux through an element of area dS, subtending a solid angle $d\omega$ at a relative distance R, is given by:

$$F(R, k'', t)d\omega\equiv(r^{-1}\mathbf{r}\cdot\mathbf{j})_{r=R}dS = (2i)^{-1}[(r\psi_S)^*(\partial r\psi_S/\partial r) - (r\psi_S)(\partial r\psi_S/\partial r)^*]_{r=R}d\omega. \tag{33}$$

From the definition (24) of the functions $\chi(r, k, t)$ it is easily seen that the flux per unit solid angle at a relative distance R, becomes:

$$F(R, k'', t)=\text{Re}C^4\left\{\left[\sum_{i=1}^{4}A_i\chi(R, k_i, t)\right]^* \times\left[\sum_{i=1}^{4}A_ik_i\chi(R, k_i, t)\right]\right\}, \tag{34}$$

where Re stands for real part of the expression (34).

From the properties of the χ's given in Secs. IV, V, we see that at $t=0$, $F(R, k'', 0)=0$, while when $t\to\infty$, the flux F tends to:

$$F(R, k'', t)\to C^4k''[(k_0^2-k''^2)^2+C^4k''^2]^{-1}, \quad (35)$$

so that the total cross section for the stationary state is given by (8).

The expression (34) for the transient scattered flux simplifies somewhat, in case the relative distance is large, i.e., if $R\gg|k''|^{-1}$, $|k_2|^{-1}$. In this case, it is seen that for any positive time $t>0$, $\chi(R, k_2, t)$, $\chi(R, -k'', t)\simeq 0$, so that the summation involved in (34) can be restricted to the values $i=1, 3$ of the indices.

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APPENDIX 1

In this appendix we shall obtain with the help of (19, 20) the time-dependent wave functions corresponding to the initial states:

$$\begin{bmatrix}(k''r)^{-1}\sin k''r\\ 0\end{bmatrix} \text{ and } \begin{bmatrix}0\\1\end{bmatrix}. \quad (36)$$

For the first of the above states, we have that the components of (17) are $\psi_1(r)=(k''r)^{-1}\sin k''r$ and $\psi_2=0$, so that the corresponding transform $F(k)$, given by (19a), is:

$$F(k)=\frac{kC^2}{k_0^2-k^2+ikC^2}\left\{(2/\pi)^{\frac{1}{2}}\int_0^\infty\left(\frac{\cos kr}{kr}+\frac{k_0^2-k^2}{kC^2}\frac{\sin kr}{kr}\right)\frac{\sin k''r}{k''r}r^2dr\right\}. \quad (37)$$

The part of (37) inside the curly bracket is clearly the ordinary Hankel transform (11) of that part of the integrand inside the round brackets. To evaluate (37), we just need the Hankel transforms of $(kr)^{-1}\sin kr$ and $(kr)^{-1}\cos kr$. We assert that these Hankel transforms are $(2\pi)^{\frac{1}{2}}k^{-1}\delta(k''^2-k^2)$ and $-(2\pi)^{\frac{1}{2}}[\pi k(k^2-k''^2)]^{-1}$ respectively, and because of the reciprocal relation (11b) that holds for Hankel transforms, our assertion will be valid if we can prove that:

$$(2/\pi)^{\frac{1}{2}}\int_0^\infty[(2\pi)^{\frac{1}{2}}k^{-1}\delta(k''^2-k^2)](k''r)^{-1}\times\sin(k''r)k''^2dk''=(kr)^{-1}\sin kr,$$

$$(2/\pi)^{\frac{1}{2}}\int_0^\infty(2\pi)^{\frac{1}{2}}[\pi k(k''^2-k^2)]^{-1}(k''r)^{-1}\times\sin(k''r)k''^2dk''=(kr)^{-1}\cos kr.$$

The first equation is obviously true, and the second will be valid if we interpret the integral in the sense of Cauchy's principal value,[17] as it can be written in the form:

$$(\pi ikr)^{-1}\int_{-\infty}^{\infty}(k''^2-k^2)^{-1}\exp(ik''r)k''dk'',$$

and the principal value of this integral, which is πi times the sum of its residues at the poles $k''=-k'$, $k''=k$, is just $(kr)^{-1}\cos kr$. We have then for $F(k)$ the form:

$$F(k)=\frac{kC^2}{k_0^2-k^2+ikC^2}\frac{(2\pi)^{\frac{1}{2}}}{k}\times\left[-\frac{1}{\pi(k^2-k''^2)}+\frac{k_0^2-k^2}{kC^2}\delta(k''^2-k^2)\right]. \quad (38)$$

Introducing this $F(k)$ in (20) we obtain the first component of the time dependent function:

$$\psi_1(r, k'', t)=\frac{k''C^2(k_0^2-k''^2)}{(k_0^2-k''^2)^2+k''^2C^4}\left[\frac{\cos k''r}{k''r}+\frac{k_0^2-k''^2}{k''C^2}\frac{\sin k''r}{k''r}\right]\times\exp(-i\tfrac{1}{2}k''^2t)-\int_0^\infty\frac{2k^2C^4\exp(-i\frac{1}{2}k^2t)}{(k_0^2-k^2)^2+k^2C^4}\times\left[\frac{\cos kr}{kr}+\frac{k_0^2-k^2}{kC^2}\frac{\sin kr}{kr}\right]\frac{kdk}{\pi(k^2-k''^2)}, \quad (39)$$

where the integral must be interpreted in the sense of Cauchy's principal value.[17]

To evaluate the integral in (39), we first simplify it by using exponential functions and extending the range of integration from $-\infty$ to ∞, so that it becomes:

$$C^2(\pi ir)^{-1}\mathrm{P}\int_{-\infty}^{\infty}k\left[\prod_{j=1}^{4}(k-k_j)\right]^{-1}\exp i(kr-\tfrac{1}{2}k^2t)dk, \quad (40)$$

where P stands for principal value of the integral, and k_j, $j=1, 2, 3, 4$ have the same meaning than in Sec. VI. We shall furthermore assume that the binding energy $E_0>0$ and that the coupling constant C^2 is small enough so that k_1, k_2 are in the lower half of the k-complex plane, and k_1 is inside the wedge as in Fig. 1. This restriction is just for the purpose of simplifying the calculation, as the final results are shown in Sec. IV, to be valid independently of the position of the poles of the scattering matrix.

We now consider the path in the complex k-plane shown in Fig. 1. As on the arcs of circle represented by dotted lines in Fig. 1, k^2 has a negative imaginary part, we see that the integrand vanishes exponentially for large values of $|k|$ on them. Also inside the contour, (which includes the circle around k_1) the integrand is a

[17] See reference 14, p. 117.

analytic function of k, so using Cauchy's theorem we obtain:

$$\mathrm{P}\int_{-\infty}^{\infty} = \pi i \,\mathrm{Res}(k=-k'') - \pi i \,\mathrm{Res}(k=k'') - 2\pi i \,\mathrm{Res}(k=k_1) + \int_{-(1-i)\infty}^{(1-i)\infty}, \quad (41)$$

where $\mathrm{Res}(k=-k'')$, etc. stand for the residues of the integrand at those values of k.

In the integral on the right of (41) we decompose the rational part of the integrand into partial fractions, so we have:

$$k\left[\prod_{i=1}^{4}(k-k_i)\right]^{-1} = \sum_{i=1}^{4} A_i(k-k_i)^{-1} \quad (42)$$

where $A_1 = k_1[(k_1-k_2)(k_1-k_3)(k_1-k_4)]^{-1}$, etc. Furthermore, we introduce a change of variable $z = k\exp(i\pi/4)$

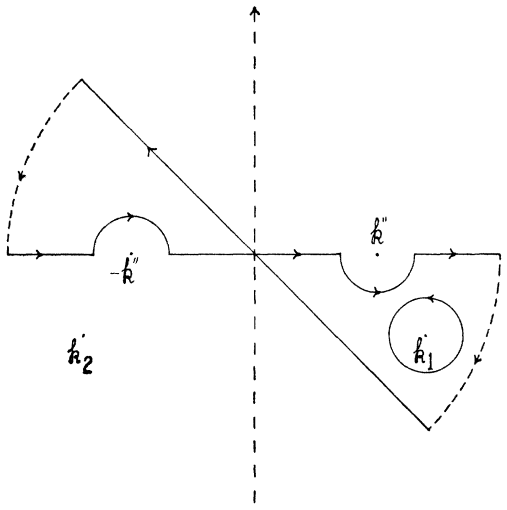

FIG. 1. Integration contour.

and we have for this integral:

$$\int_{-(1-i)\infty}^{(1-i)\infty} = \sum_{j=1}^{4} A_j \int_{-\infty}^{\infty} (z-z_j)^{-1}\exp(\lambda z - \nu z^2)dz \equiv \sum_{j=1}^{4} A_j F(\nu, \lambda, z_j), \quad (43)$$

where $\lambda = r\exp(i\pi/4)$, $\nu = (t/2)$, $z_j = k_j\exp(i\pi/4)$. Now, the functions $F(\nu, \lambda, z_j)$ defined by the integrals in (43) can be easily evaluated, either by differentiating them with respect to λ and solving the differential equation that appears, or with the help of a table of Fourier transforms.[18] The function $F(\nu, \lambda, z_j)$ takes then the form:

$$F(\nu, \lambda, z_j) = \exp(\lambda z_j - \nu z_j^2)\pi i \times\{\mathrm{erf}[(2i\nu^{\frac{1}{2}})^{-1}(\lambda - 2\nu z_j)] \pm 1\}, \quad (44)$$

where the + sign is used when the imaginary part of $z_j > 0$ and the − sign when it is <0. The function $\mathrm{erf}(z)$ is the error integral of (25).

With the help of (44) we can evaluate (43) using the + sign in (44) for the poles k'', k_1, and the − sign for $-k''$, k_2. From (43) and the values of the residues of the integrand in (41), we obtain finally:

$$\psi_1(r, k'', t) = (k''r)^{-1}\sin k''r\exp(-i\tfrac{1}{2}k''^2 t) - C^2 r^{-1}\sum_{i=1}^{4} A_i\chi(r, k_i, t), \quad (45)$$

where $\chi(r, k_i, t)$ is the function defined by (24). Introducing this value in (22a), we obtain the expression for the first component of $\Psi(\mathbf{k}'', t)$ given by (23).

If we now consider the second state in (36), we see that for this state the components of (17) are $\psi_1(r) = 0$, $\psi_2 = 1$ so that the corresponding transform $F(k)$ is by (19a) just:

$$F(k) = (2/\pi)^{\frac{1}{2}}C'(k_0^2 - k^2 + ikC^2)^{-1}. \quad (46)$$

The first component of the corresponding time dependent function, which is now $\psi_{12}(\mathbf{r}, t)$, is obtained by introducing (46) in (20), and we have:

$$\psi_{12}(r, t) = (2\pi^2 C')^{-1}\int_0^{\infty} \frac{k^2 C^4\exp(-i\frac{1}{2}k^2 t)}{(k_0^2-k^2)^2 + k^2C^4} \times\left[\frac{\cos kr}{kr} + \frac{k_0^2 - k^2}{kC^2}\frac{\sin kr}{kr}\right]kdk. \quad (47)$$

This integral has a form similar to the one that appears in (39), except that the factor $(k^2-k''^2)^{-1}$ is not present, so that there are no poles at $k = \pm k''$. The evaluation of (47) can be made along similar lines than in the preceeding case, and we only need to eliminate the indentations of the contour at $k = \pm k''$, as there is no need to consider principal values here. The result of the integration is given in (27a).

APPENDIX 2

We shall summarize here some of the asymptotic properties of the error integral function $\mathrm{erfc}(z)$, and derive from them the asymptotic behavior of $\chi(r, k, t)$ defined by (24), when $t \to 0$ and $t \to \infty$.

It is known[14] that the error integral can be expressed in terms of confluent hypergeometric functions in the form:

$$\mathrm{erfc}(z) = (\pi z)^{-\frac{1}{2}}\exp(-\tfrac{1}{2}z^2)W_{-\frac{1}{2},\,\frac{1}{4}}(z^2) \quad (48)$$

and from the asymptotic behavior of these functions[14] we can obtain directly that for $|z| \to \infty$,

$$\mathrm{erfc}(z) \to \pi^{-\frac{1}{2}}z^{-1}\exp(-z^2), \quad \text{if } -\pi/2 < \arg z < \pi/2. \quad (49)$$

[18] G. E. Campbell and R. M. Foster, *Fourier Integrals for Practical Applications* (D. Van Nostrand Company, Inc., New York, 1948), Formula 728.5.