$(1-I/\epsilon)^2$  in the remaining summations should act to reduce the value of F as I increases.

In conclusion, it seems rather likely that Fshould generally be of the order of magnitude of  $\frac{1}{3}$  to  $\frac{1}{2}$ .6

<sup>6</sup> The ionizing action of comparatively energy-rich but slow ions, of velocity close to that of molecular valence

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I wish to thank Dr. J. H. Curtiss and Dr. C. Eisenhart for helpful discussions and advice on the statistical treatment and Dr. D. Blackwell for discussing his results with me prior to publication.

electrons, constitutes an exceptional case for the determination of both  $\epsilon$  and F;  $\epsilon$  may become much larger than 30–35 ev, and F may approach 1.

VOLUME 72, NUMBER '1

JULY 1, 1947

#### Higher Angular Momenta and Long Range Interaction in Resonance Reactions

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The results of two preceding articles on the energy dependence of the reaction and scattering cross sections are generalized. As before, the configuration space is divided into two parts. In the internal region or reaction zone there is no restriction on the type of interaction between the particles. In the external region, on the other hand, the interaction takes place between the colliding or separating particles without changing their structure (wave function). The present article deals with a more general situation than the preceding ones, first by allowing for an interaction, although only of a restricted type, outside the reaction zone. The most common type of interaction which plays a role outside the reaction zone is the electrostatic interaction of the colliding or separating particles. In

# I. INTRODUCTION AND SUMMARY

**'**HE present treatment of the representation of the scattering and reaction cross sections differs from that given in two previous papers<sup>1a, b</sup> in that it divides the problem of finding a stationary solution of the quantum-mechanical equations into two steps. The first step is taken in Section III; Section II is devoted to the introduction of several definitions and a few mathematical preliminaries. In Section III an expression is obtained for the value which the wave function assumes on the surface S separating the internal and external regions,<sup>2</sup> in terms of the addition, the present article does not restrict the angular momentum of the particles to zero, but permits the treatment of arbitrary angular momenta. The cross sections are expressed in well-known fashion in terms of the collision matrix U which is, of course, independent of the size of the internal region.  $\mathfrak{U}$ , in its turn, is expressed by the  $\mathfrak{R}$ matrix ((35) and (38)) and the quantities  $\omega$ ,  $\mathfrak{B}$ , and  $\mathfrak{C}$ describing the interaction in the external region.  $\Re$  as function of energy is given by (24), and a number of properties of this function are enumerated. None of the quantities  $\mathfrak{N}, \omega, \mathfrak{B}$ , and  $\mathfrak{C}$  are strictly independent of the size of the internal region, although the combination (38), i.e., the collision matrix, of course, is.

normal derivative of the wave function on that surface. The essential content of this section may be described as follows. A complete set of orthonormal functions  $X_{\lambda}$  is defined in the internal region by means of an Hermitean boundary value problem. The  $X_{\lambda}$  are those solutions of the wave equation which satisfy the boundary condition that their normal derivatives vanish at the boundary S of the internal region. If an arbitrary stationary-state wave function,  $\varphi$ , associated with the energy E, is expanded in terms of the  $X_{\lambda}$  the expansion coefficients are found to be  $\gamma_{\lambda}/(E_{\lambda}-E)$  where  $\gamma_{\lambda} = \int X_{\lambda}^* (\partial \varphi/\partial n) dS$ . The  $E_{\lambda}$ is the characteristic value associated with  $X_{\lambda}$ ,  $\partial \varphi / \partial n$  denotes the normal derivative; the integral is to be extended over the boundary surface S. As a result, the value of  $\varphi$  is given by

$$\varphi = \sum_{\lambda} \frac{\gamma_{\lambda}}{E_{\lambda} - E} X_{\lambda} = \sum_{\lambda} \frac{\int X_{\lambda}^{*} (\partial \varphi / \partial n) dS}{E_{\lambda} - E} X_{\lambda}.$$
 (1)

<sup>&</sup>lt;sup>1a</sup> E. P. Wigner, Phys. Rev. **70**, 15 (1946). <sup>1b</sup> E. P. Wigner, Phys. Rev. **70**, 606 (1946). Professors J. Schwinger and V. Weisskopf have kindly informed us that they have recently obtained results which closely parallel those of the present paper.

<sup>&</sup>lt;sup>2</sup> Most of the notions (such as internal and external region, etc.) used in this paper were formulated by the writers in 1940 for a review article, the publication of which was postponed because of the war. It will appear shortly in another journal.

Since  $\gamma_{\lambda}$  depends only on the normal derivative of  $\varphi$  on *S*, Eq. (1) constitutes a relation between the value and the normal derivative of  $\varphi$  on *S*. If both  $\varphi$  and  $\partial \varphi / \partial n$  are expanded into an orthogonal system, the integral operator defined by (1) goes over into the matrix  $\Re$  which has the same significance as the  $\Re$  of reference 1b. The expression obtained there for  $\Re$  is rederived here, and it is shown that the constant matrix  $\Re_{\infty}$ vanishes. The  $\Re$  matrix plays a central role, and since its form is given implicitly by (1), this equation contains, in a sense, the essential content of the present paper.

Although the boundary condition on the  $X_{\lambda}$ , which is actually used in Section III, is somewhat more complicated than the one given above (vanishing normal derivative on S), the relation which is derived between value and normal derivative of  $\varphi$  is formally identical with (1). The reasons for the choice of the particular boundary conditions employed will become apparent later, but it should be emphasized here, perhaps, that there is a certain arbitrariness in the choice of these conditions (and hence of the  $X_{\lambda}$  and  $E_{\lambda}$ ) and that the ones used may not always be the most suitable ones.

Section IV deals with the second step for obtaining an expression for the scattering and reaction cross sections. It consists in obtaining that consistent set of values and derivatives of the wave function on the surface S, the continuation of which into the external region gives the asymptotic form which corresponds to an experiment to determine the scattering and reaction cross sections. While Section III deals with the condition that the values and derivatives of the wave function on the surface dividing the internal and external regions be continuable into the internal region, Section IV gives the condition that the continuation into the external region give the correct asymptotic behavior. One can also say that Section IV gives Heisenberg's S matrix or Wheeler's collision matrix<sup>3</sup> in terms of the  $\Re$ matrix obtained in Section III.

In Section V some general aspects of the results of the preceding sections are discussed. Also the form of the one-level resonance formula, which follows when all terms of Eq. (1), excepting one, can be assumed to be independent of energy, is derived.

#### II. THE INTERNAL AND EXTERNAL REGIONS OF CONFIGURATION SPACE

Qualitatively, the internal region of the configuration space is characterized by the condition that all particles are relatively close together, the external region by the requirement that the system is well separated into two sub-systems. The forces between these sub-systems are either entirely absent or, if present, of such a nature that the internal structure of the sub-systems is not affected. The boundary between the internal and external regions will be called S.

For a more exact and quantitative formulation we must start with a few preliminaries.<sup>4</sup> Let us consider a typical nuclear reaction

$$\operatorname{Li}^{7} + \operatorname{H}^{1} \longrightarrow \begin{cases} \operatorname{Li}^{7} + \operatorname{H}^{1} \\ \operatorname{Be}^{7} + n \\ \operatorname{Li}^{6} + \operatorname{H}^{2} \\ \operatorname{He}^{4} + \operatorname{He}^{4} \end{cases}$$
(A)

The various reaction products which appear on the right side will be called "alternatives." Thus  $He^4 + He^4$  is an alternative of the reaction (A). The pair Li<sup>6</sup>+H<sup>2</sup> represents not one but several alternatives, corresponding to the different possible states of polarization of the spins of Li<sup>6</sup> and of  $H^2$ . Since both these spins are 1, the total possible number of polarizations is  $3 \times 3 = 9$ , and the third pair of (A) represents 9 alternatives. The pair  $Li^7 + H^1$  can be formed so that  $Li^7$  is in the normal state or in the first excited state. In the former case, the spin is  $\frac{3}{2}$ , giving  $4 \times 2 = 8$ alternatives, in the latter case probably  $\frac{1}{2}$ , giving  $2 \times 2 = 4$  alternatives. The same holds of the Be<sup>7</sup>+n pair. Altogether, the reaction (A) is, in the energy region in which the above described end products are possible, an (8+4)+(8+4)+9+1=34 alternative reaction. It is desirable, furthermore, to consider, along with the reactions (A), all the reactions in which any of the end products of (A) is the initial state. These are, in the present instance,  $34 \times 34$  reactions.

<sup>&</sup>lt;sup>8</sup> J. A. Wheeler, Phys. Rev. 52, 1107 (1937); W. Heisenberg, Zeits, f. Physik 120, 513, 673 (1943); C. Moller, I. D. Kgl. Danske Vid. Sels. Mat. Phys. Med. 23, 1 (1945).

<sup>&</sup>lt;sup>4</sup> The definition of "alternatives" which follows is not quite the same as that used in Proc. Nat. Acad. **32**, 302 (1946).

Some of these are, of course, not real reactions but scattering processes.

There is a certain arbitrariness in the definition of the states of polarization of the pair  $Li^6+H^2$ , for instance. We shall use the following convention: From the spin wave functions of the pair we build such a linear combination that the composite angular momentum of the pair is definite. Similarly, the component of this angular momentum in a given direction (usually the Zdirection) shall have a definite value. The different alternatives will be distinguished by two indices, s and  $\nu$ . The former determines the nature and state of excitation of the pair together with the angular momentum resulting from the spins of the pair. The magnitude of this resultant angular momentum will be denoted by  $j_s$ . The index  $\nu$  gives the component of this angular momentum in the Z direction. Neither  $j_s h$  nor  $\nu h$  is necessarily the total angular momentum or the Z component of total angular momentum of the system because they do not include the angular momentum of the motion of the nuclei, which forms the pair s, with respect to their common center of mass. This is, to be sure, zero in a head-on collision, but is finite in general.

The product of the normalized wave functions of the two nuclei He<sup>4</sup>+He<sup>4</sup> will be denoted by  $\psi_{s0}$  if *s* designates the pair He<sup>4</sup>+He<sup>4</sup>. In general, the  $\psi_{s\nu}$  will not be a simple product but a linear combination of such products, which will be assumed, in all cases, to be normalized:

$$\int |\psi_{s\nu}|^2 di_s = 1, \qquad (2)$$

where  $di_s$  denotes integration over the internal coordinates of the nuclei which make up the pair s. It is probably unnecessary to mention that  $\psi_{s\nu}$ is independent of the energy with which these particles collide or separate. In addition to (2), one can assume<sup>5</sup> that  $\psi_{s\nu}$  is real in the sense that

$$K\psi_{s\nu} = -i^{2\nu}\psi_{s-\nu},\tag{3}$$

where K implies the transition to the conjugate imaginary and multiplication with the imaginary spin operator  $(\sigma_{\nu})$  of all the elementary particles in the two nuclei. The point of the normalization (3) is that the scalar product of two functions, normalized by (3), is real. It is zero if the *j* value of the two functions is different, or if their  $\nu$ values are different. If the two *j* and  $\nu$  are the same, the scalar product is independent<sup>6</sup> of  $\nu$  and one can argue<sup>5</sup>

$$(f_{\nu}, g_{\nu}) = (Kg_{\nu}, Kf_{\nu}) = (i^{2\nu}g_{-\nu}, i^{2\nu}f_{-\nu})$$
$$= (g_{-\nu}, f_{-\nu}) = (f_{-\nu}, g_{-\nu})^{*}, \quad (4)$$

However, because of the last statement  $(f_{\nu}, g_{\nu})$  is also equal to  $(f_{-\nu}, g_{-\nu})$ ; it is equal to its conjugate complex and hence real.

We now can state more accurately what we mean by external and internal parts of the configuration space. In the external part, the most general solutions of the quantum-mechanical equations with a definite energy are linear combinations of functions of the form

$$F_s(r_s, \Omega_s)\psi_{s\nu}(i_s). \tag{5}$$

In this,  $\psi_{sv}$  is one of the functions described above, *i*<sub>s</sub> denoting the internal coordinates of the nuclei which make up the pair *s*. The *r*<sub>s</sub> and  $\Omega_s$  denote length and direction of the vector connecting the nuclei of the pair *s*. In other words, the system is in one of the alternate states (A) which the reaction can yield. The *F*<sub>s</sub> is a solution of the Schrödinger equation in three-dimensional space with the potential which acts between the pair *s*. The external region is so defined that the interaction of the nuclei which make up the different pairs can already be represented by a potential. Clearly, *F*<sub>s</sub> is independent of *v*. The internal region is the remaining part of configuration space.

It may be well to remark here that the size of the internal region is not defined; the above gives it only a minimum size. It is always possible to add to the internal region part of the configuration space which could be in the external region. One will try, however, for reasons which will become clear later, to make the internal region as small as possible. It should be noted, furthermore, that the size of the internal region is a

<sup>&</sup>lt;sup>5</sup> E. P. Wigner, Göttinger Nachr. **31**, 546 (1932). Actually, the normalization used in this paper is somewhat awkward since (3) implies that a function  $\psi_{s0}$ , which is real in the sense (3), is imaginary in the usual sense. However, this is purely a matter of convention and plays, in fact, very little part in the following. The spins of the particles make the following derivation appear much more complicated than it actually is. If the spins of all the particles participating in the reaction were zero, all  $j_s$  would vanish;  $s(j_s, l)_{Jym} = s(0, l)_{J0m} = \delta_{lJ}$  would hold, and all formulae would be considerably simplified.

<sup>&</sup>lt;sup>6</sup> E. P. Wigner, *Gruppentheorie* (Edwards Brothers, Ann Arbor, 1944), Chapter XII.

function of the energy range which one considers. With increasing total energy of the system, the number of excited states of the product nuclei which one has to take into account will also increase, and so will the distance at which these excited nuclei interact intimately. At the energy at which three or more free product nuclei can be formed, the present considerations lose validity.

Since  $F_s(r_s, \Omega_s)$  obeys a second-order partial differential equation in three-dimensional space, it is completely determined in that part of the three-dimensional space which corresponds to the external region, if its value and normal derivative at the surface S of that region are given. It is practical, therefore, to choose surfaces  $r_s = a_s$ to form the boundary between these regions. Since, furthermore, the Schrödinger equation for  $F_s$  has a spherically symmetric potential, its general solution is a linear combination of functions of the form

$$r_s^{-1} \mathbb{S}_{sl}(r_s) P_{lm}(\Omega_s)$$
 and  $r_s^{-1} \mathbb{C}_{sl}(r_s) P_{lm}(\Omega_s)$ . (6)

The  $P_{lm}(\Omega_s)$  are the well-known spherical harmonics giving, to the relative motion of the pair s, the value  $l\hbar$  for the magnitude of the angular momentum and the value  $m\hbar$  for its Z-component. We assume that the  $P_{lm}$  are normalized if integrated over the surface of the unit sphere, and that they obey a condition similar to (3):

$$P_{lm}(\Omega)^* = -(-)^m P_{l-m}(\Omega).$$
<sup>(7)</sup>

The  $S_{sl}(r_s)$  and the  $C_{sl}(r_s)$  are solutions of the radial Schrödinger equation which applies to  $F_s$ . These are chosen so that at  $r_s = a_s$ ,

$$S_{sl}(a_s) = 0, \qquad C_{sl}(a_s) = (M_s/\hbar)^{\frac{1}{2}},$$
$$\frac{d}{dr_s}S_{sl}(a_s) = \left(\frac{M_s}{\hbar}\right)^{\frac{1}{2}}, \quad \frac{d}{dr}C_{sl}(a_s) = -\frac{l}{a_s}\left(\frac{M_s}{\hbar}\right)^{\frac{1}{2}}. \quad (8)$$

 $M_s$  is the reduced mass of the pair s. Evidently, S and C depend not only on the energy but also on the position  $r_s = a_s$  of the boundary between internal and external regions;  $P_{lm}$  is independent of both. The notations S and C were chosen to manifest the analogy with the functions  $(M/\hbar)^{\frac{1}{2}}k^{-1}\sin k(r-a)$ , and  $(M/\hbar)^{\frac{1}{2}}\cos k(r-a)$  into which S and C go over if the angular momentum l=0, and if there are no forces acting in the external region between the particles of the pair s. The boundary conditions (8) were chosen with a view to making the behavior of S and C simple for small kr. For small kr, the two simplest solutions of the radial wave equation behave as  $r^{l+1}$  and  $r^{-l}$ . The latter satisfies the boundary condition for C. The corresponding boundary condition for S would read  $S_{sl}(a_s) = (M_s/h)^{\frac{1}{2}}a_s/(l+1)$ . Since this is a small quantity, it was replaced by 0, which also gave some formal simplifications.

The last preliminary step is the formation of wave functions which have definite total angular momenta which include both the spins of the particles of the pair *s* and the momentum of their relative motion. This can be done by the coefficients  $s_{Jym}^{(jl)}$ , well known from the vector-addition model<sup>7</sup>

$$\mathfrak{D}_{sl\mu}{}^{J}(r_{s}, \Omega_{s}, i_{s}) = \sum_{m} s(j_{s}, l) J_{\mu-mm} r_{s}^{-1} \\ \times \mathfrak{S}_{sl}(r_{s}) P_{lm}(\Omega_{s}) \psi_{s\mu-m}(i_{s}), \qquad (9) \\ \mathfrak{V}_{sl\mu}{}^{J}(r_{s}, \Omega_{s}, i_{s}) = \sum_{m} s(j_{s}, l) J_{\mu-mm} r_{s}^{-1} \\ \times \mathfrak{C}_{sl}(r_{s}) P_{lm}(\Omega_{s}) \psi_{s\mu-m}(i_{s}).$$

The symbols  $\mathfrak{D}$  and  $\mathfrak{V}$  were chosen because  $\mathfrak{D}$  has a finite derivative,  $\mathfrak{V}$  a finite value on the boundary of the internal and external regions. Both  $\mathfrak{D}$ and  $\mathfrak{V}$  are solutions of the quantum-mechanical equation in the external region for a stationary state with energy E. They represent states with a total angular momentum J, and a Z component  $\mu$  (zero linear momentum), and they both are real in the sense that they satisfy the equations,

$$K \mathfrak{D}_{sl\mu} = -i^{2\mu} \mathfrak{D}_{sl-\mu}, \quad K \mathfrak{V}_{sl\mu} = -i^{2\mu} \mathfrak{V}_{sl-\mu}.$$
 (10)

As a result of the normalization of  $S_{sl}$  and  $C_{sl}$  as given by (8), it follows that on the surface S

$$\frac{\partial \mathfrak{D}_{sl\mu}{}^J}{\partial r_s} = \mathfrak{V}_{sl\mu}{}^J \text{ (on } S\text{).}$$
(11)

A second relation which will be useful in the next section is

$$\int \mathfrak{V}_{sl\mu}{}^{J*}\mathfrak{V}_{s'l'\mu}{}^{J}dS = \delta_{ss'}\delta_{ll'}(M_s/\hbar), \quad (12)$$

which is a consequence of (8), the orthogonality

<sup>&</sup>lt;sup>7</sup> Reference 6, Chapter XVII, Section 6. The number of alternatives, as defined in the paper of reference 4, is the number of different pairs s, l for a given J. It is also the number of dimensions of the matrix  $\Re$  which will be defined in Section III.

of the  $P_{lm}$  and the  $\psi_{sv}$ , and the unitary character of the *s*-coefficients (Chapter XVII of reference 6).

It may be well to repeat that the  $s(j, l)_{J\mu-mm}$ , the  $P_{lm}$ , and the  $\psi_{s\nu}$  are independent both of the energy E and also of the location  $a_s$  of the boundary between external and internal regions. The  $S_{sl}$  and  $C_{sl}$  depend on both. This completes the preliminary work for the rest of the development.

### III. THE R MATRIX

The general solution of the quantum-mechanical equations in the external region is a linear combination of the  $\mathfrak{D}$  and  $\mathfrak{V}$  of (9) with arbitrary coefficients. The purpose of the present section is to derive relations between these coefficients which guarantee that the solution can be continued into the internal region to give a singularity-free solution of the equations in that region also. Since the coefficients of the D determine the derivative of the wave function on the surface Swhich separates the external and internal regions, and since the coefficients of the v do likewise for the value of the wave function, the relations between these coefficients give also the relations between derivative and value of the wave function which must hold on the surface S in order that the continuation of the wave function into the internal region be possible.

Since the quantum-mechanical equations are linear, it is sufficient to determine a set of basic solutions out of which the general solution, and in particular the one fitting the experimental conditions, can be obtained by superposition. We chose these wave functions so that they represent states with definite values of the total angular momentum J and its Z-component  $\mu$ . These will be, in the external region, superpositions of the  $\mathfrak{D}$  and  $\mathfrak{V}$  with a single J and  $\mu$ . We may drop, therefore, for this section, the superscript J.

There are as many linearly independent states with definite J and  $\mu$  (and definite energy) as the indices s and l can assume values. (This is equal to the number of alternatives, as defined in reference 4. The index l can assume every integer value between  $|J-j_s|$  and  $J+j_s$ .) We shall define our basic solutions so that they contain only one  $\mathfrak{D}$ ; the coefficients of the  $\mathfrak{V}$  are then determined:

$$\varphi_{sl\mu} = \mathfrak{D}_{sl\mu} + \sum_{s'l'} R_{sl;s'l'} \mathfrak{U}_{s'l'\mu}.$$
(13)

Equation (13) holds in the external region but  $\varphi$  can be continued into the internal region.  $\Re$  depends on the energy and on J but is independent of  $\mu$ . Applying K to (13) one obtains by (10)

$$-K\varphi_{sl\mu} = i^{2\mu}\mathfrak{D}_{sl-\mu} + \sum_{s'l'} R_{sl;s'l'} * i^{2\mu}\mathfrak{V}_{s'l'-\mu}.$$
 (14)

Since  $K\varphi$  is also a solution of the quantum-mechanical equations,<sup>5</sup> (14) is evidently  $i^{2\mu}\varphi_{sl-\mu}$ , and since  $\Re$  is independent of  $\mu$ ,

$$R_{sl;\,s'l'}^* = R_{sl;\,s'l'},\tag{15}$$

i.e., the elements of  $\Re$  are real.

The object of this section is to determine the coefficients R as functions of the energy. For this purpose we consider those solutions  $X_{\lambda\mu}$  of the quantum-mechanical equations in the internal region which satisfy the boundary conditions at the surface S,

$$-\frac{l+1}{a_s}\int X_{\lambda\mu}*P_{lm}(\Omega_s)\psi_{s\nu}dS$$
$$=\int \operatorname{grad}_n X_{\lambda\mu}*P_{lm}(\Omega_s)\psi_{s\nu}dS,$$

where grad<sub>n</sub> is the component of the gradient normal to S. The  $X_{\lambda\mu}$  thus satisfy the same boundary condition as the  $\mathcal{V}_{sl\mu}$ . The characteristic value problem for the  $X_{\lambda\mu}$  is Hermitean, and  $X_{\lambda\mu}$  can be assumed to form a complete set of orthonormal functions. Furthermore, since the problem defining the  $X_{\lambda\mu}$  does not prefer any direction in ordinary space, a J and  $\mu$  can be defined and  $X_{\lambda\mu}$  assumed to be real in the sense of (3). The characteristic value of  $X_{\lambda\mu}$  will be denoted by<sup>8</sup>  $E_{\lambda}$ .

<sup>&</sup>lt;sup>8</sup> It should be noted that this is a well-defined boundary value problem even though some of the  $E_{\lambda}$  fall outside the energy region in which the formulae are valid. That region applies to E and not to the  $E_{\lambda}$ . P. L. Kapur and R. Peierls, Proc. Roy. Soc. A166, 277 (1937) also introduce an orthogonal system to express the wave functions in what corresponds to our internal region. As a result, there are many common features between their treatment and ours. However, their boundary condition depends on the energy so that they use, in effect, a different set of expanding func-tions for every energy. As a result, the "constants" in their equations are only approximately independent of energy, and this dependence makes it quite difficult to derive e.g., the proportionality of the particle widths in the one-level formula to the velocity. The complicated nature of the relation of their constants to those used here is illustrated in Fig. 2 of reference 1b. On the other hand, their constants have a closer relation to the observable cross sections than ours,

If one applies Green's theorem to  $\varphi_{sl\mu}$  and  $X_{\lambda\mu}$ , the terms in the surface integral which contain the  $\mathcal{V}$  drop out by virtue of the boundary condition imposed on the  $X_{\lambda\mu}$ , and one has

$$-\frac{\hbar^2}{2M_s}\int X_{\lambda\mu}^* \frac{\partial}{\partial r_s} \mathfrak{D}_{s\,l\mu} dS$$
$$= (E - E_{\lambda}) \int X_{\lambda\mu}^* \varphi_{s\,l\mu} dI. \quad (16)$$

The last integral has to be extended over the internal region. The left side assumes<sup>9</sup> that only those  $\mathfrak{D}$  and  $\mathfrak{V}$  have to be considered on the part of S which is given by  $r_{s'}=a_{s'}$  which have the first index s'.

Introducing (11) into (16) we obtain for its left side

$$-\frac{\hbar^2}{2M_s}\int X_{\lambda\mu}^* \mathfrak{V}_{sl\mu} dS = -\left(\frac{\hbar}{2}\right)^{\frac{1}{2}} \gamma_{\lambda sl}; \quad (17)$$

the right side defines the  $\gamma$  which is independent of E (and of  $\mu$ ) and, as the scalar product of two real functions, is also real because of (4). Since the  $X_{\lambda\mu}$  form an orthonormal set, we can write for the internal region

$$\varphi_{sl\mu} = \sum_{\lambda} A_{sl\lambda} X_{\lambda\mu}, \qquad (18)$$

whence (16) gives

$$A_{sl\lambda} = \left(\frac{\hbar}{2}\right)^{\frac{1}{2}} \frac{\gamma_{\lambda sl}}{E_{\lambda} - E}.$$
 (19)

The energy dependence of the  $\Re$ -matrix could now be obtained by a development which closely parallels that of reference 1. In this method a second application of Green's theorem to the functions  $\varphi_{sl\mu}$  and  $\varphi_{s'l'\mu'}$ , for the different energies E and E', is made. The evaluation of the surface integral involved is obtained by neglecting on that part of the surface which is given by  $r_t = a_t$ , all  $\mathfrak{D}$  and  $\mathfrak{V}$  terms the first index of which is not t. The result of this procedure,

$$R_{sl;s'l'} = \sum_{\lambda} \frac{\gamma_{\lambda sl} \gamma_{\lambda s'l'}}{E_{\lambda} - E} + R_{sl;s'l'}(\infty) \qquad (20)$$

where  $R_{sl;s'l'}(\infty)$  is an arbitrary real-symmetric matrix independent of the energy, is a generalization of Eq. (33a) of reference 1b.

The  $\Re$ -matrix may also be obtained by the requirement that  $\varphi_{sl\mu}$  be continuous at the boundary S. This condition leads to the above equation with  $R(\infty) = 0$ . Since  $\mathfrak{D}$  is zero at the boundary we have as the condition for continuity from (13), (18), and (19)

$$\left(\frac{\hbar}{2}\right)^{\frac{1}{2}}\sum_{\lambda}\frac{\gamma_{\lambda sl}}{E_{\lambda}-E}X_{\lambda\mu}=\sum_{s^{\prime\prime}l^{\prime\prime}}R_{sl;s^{\prime\prime}l^{\prime\prime}}\mathfrak{V}_{s^{\prime\prime}l^{\prime\prime}\mu}.$$
 (21)

If both sides are multiplied by  $-(\hbar^2/2M_s)\mathcal{U}_{s'l'\mu}^*$ and integrated over the boundary S we have, on making use of (17),

$$-\left(\frac{\hbar}{2}\right)\sum_{\lambda}\frac{\gamma_{\lambda sl}\gamma_{\lambda s'l'}}{E_{\lambda}-E} = -\frac{\hbar^2}{2M_{s'}}\sum_{s''l''}R_{sl;s''l''}$$
$$\times \int \mathcal{V}_{s''l''\mu}\mathcal{V}_{s'l'\mu}^*dS. \quad (22)$$

The orthogonality properties of the  $\mathcal{U}_{sl\mu}$ , (12), reduce this equation to

$$R_{sl;s'l'} = \sum_{\lambda} \frac{\gamma_{\lambda sl} \gamma_{\lambda s'l'}}{E_{\lambda} - E}.$$
 (23)

Note that  $\Re$  in addition to being real is symmetric. In the matrix notation used in reference 1 Eq. (23) becomes<sup>10</sup>

$$\Re(E) = \sum_{\lambda} \frac{\gamma_{\lambda} \times \gamma_{\lambda}}{E_{\lambda} - E}.$$
 (24)

Although hardly any assumptions enter into (24), the class of functions which can be brought into the form (24) has some remarkable properties. Let us consider first the case of a single alternative reaction with spins zero in which case both the matrices  $\Re$  and the vectors  $\gamma$  be-

<sup>&</sup>lt;sup>9</sup> This is the condition which gives the effective lower limit to the size of the internal region. It shows, in particular, that the size of the internal region becomes increasingly large as one approaches the energy at which a new pair of reaction products is about to become energetically possible. This case needs, therefore, separate investigation.

<sup>&</sup>lt;sup>10</sup> Concerning the derivation given above, which leads to the more specific formula (23) or (24), it is well to remark that it is based on the convergence of the series of (18) at the boundary S. One can prove the convergence of this series under certain simplifying restrictions, and we are convinced that (18) converges also in general. We point this out specifically because it is easy to see that the series of the normal derivatives of the right side of (18) does not converge to the derivative of the left side. In finding the present derivation the main difficulty was to realize that (18) is a correct equation even at the surface S but that the equation obtained by differentiating it term by term is incorrect.

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come numbers. Then  $\Re(E)$  has the following properties:<sup>11</sup>

(i) All its odd derivatives are positive wherever they exist (i.e., except at the points  $E_{\lambda}$ ).

(ii) All its derivatives satisfy the inequality

$$(R^{(n+m)}/(n+m)!)^{2}$$
  
 $\leq R^{(2n+1)}R^{(2m-1)}/(2n+1)!(2m-1)!$ 

except at the points  $E_{\lambda}$ .

It is not known whether every real function which satisfies these conditions can be brought into the form (24). If there are several alternatives,  $\Re$  is a matrix and (i) and (ii) hold for the quadratic form of  $\Re$  with any real energyindependent vector.

Although it may be a mere mathematical curiosity, it will be mentioned that if  $\Re$  has the form (24), the function

$$\frac{\Re}{1+\alpha\Re} \tag{25}$$

also can be brought into that form. In addition, of course, any linear combination of functions of the form (24) with positive coefficients has again that form.

#### IV. CONNECTION BETWEEN $\Re$ AND THE COL-LISION MATRIX

The last two equations, (23) and (24), contain the major result of the present article: they give in conjunction with (13) the connection between the derivative and the value of the wave function on the surface S which must hold if the wave function is to be continuable into the internal region. The real constants which appear in (23), i.e., the  $E_{\lambda}$  and the  $\gamma_{\lambda}$ , are energy independent although they differ for different total angular momenta J. In order to bring this out, the  $\Re$  will be given an upper index J henceforth.

As far as the present derivation is concerned, it seems that the above constants can be entirely arbitrary. It is possible, however, that this is not the case and that there are relations between them (similar to the sum rules) which are always fulfilled.

The purpose of this section is to express the scattering and reaction cross sections in terms of  $\mathfrak{R}^J$ . For this purpose, we need the asymptotic behavior of the solutions  $\mathfrak{D}$  and  $\mathfrak{V}$  which are defined in (9) and occur in (13). Because of the real character of the  $\mathfrak{S}$  and  $\mathfrak{C}$  we can write

$$S_{sl}(r_s) \rightarrow \frac{1}{2}i(A_{sl}v_s^{-\frac{1}{2}}\exp(-ik_sr_s) - A_{sl}^*v_s^{-\frac{1}{2}}\exp(ik_sr_s)),$$

$$C_{sl}(r_s) \rightarrow \frac{1}{2}(B_{sl}\omega_{sl}^*v_s^{-\frac{1}{2}}\exp(-ik_sr_s) + B_{sl}\omega_{sl}v_s^{-\frac{1}{2}}\exp(ik_sr_s)).$$
(26)

The *A*, *B*, and  $\omega$  are energy-dependent constants; *B* and  $\omega$  can be assumed to be positive real, and of modulus 1, respectively. *A* is complex in general. The reason for the notation adopted in (26) will be apparent later. The  $v_s = \hbar k_s/M_s$  is the relative velocity of the particles of the pair *s* at infinity, so that the  $v_s^{-\frac{1}{2}} \exp(\pm ik_s r_s)$  corresponds to unit flux. Since the  $S_{sl}$  and  $C_{sl}$  satisfy the same second-order differential equation,  $C_{sl}dS_{sl}/dr_s$  $-S_{sl}dC_{sl}/dr_s$  is independent of  $r_s$ . As the value of this expression is  $M_s/\hbar$  at  $r_s = a_s$  (Eq. (8)), it follows that

$$B_{sl}\omega_{sl}A_{sl} + B_{sl}\omega_{sl}^*A_{sl}^* = 2.$$
 (27)

The  $B_{sl}$ ,  $\omega_{sl}$ , and  $A_{sl}$  may be considered as diagonal elements of the diagonal matrices  $\mathfrak{B}$ ,  $\omega$ , and  $\mathfrak{A}$ . They will play roles similar to the various powers of k in earlier articles.<sup>1</sup> With this notation, (27) reads

$$\mathfrak{B}\omega\mathfrak{A} + \mathfrak{B}\omega^*\mathfrak{A}^* = 2, \qquad (28)$$

so that one can also write

$$\mathfrak{B}\omega\mathfrak{A} = 1 - i\mathfrak{C}, \quad \mathfrak{B}\omega^*\mathfrak{A}^* = 1 + i\mathfrak{C}, \quad (29)$$

where  $\mathfrak{G}$  is a real diagonal matrix. It will be assumed that the  $\mathfrak{S}$  and  $\mathfrak{C}$  are known functions of r. Hence the  $\mathfrak{A}$ ,  $\omega$ , and  $\mathfrak{B}$  will be energy dependent but known quantities. We shall further use the abbreviations  $I_{svlm}$  and  $E_{svlm}$  for those solutions of the quantum-mechanical equations in the external region which correspond to incident and emerging waves. Their asymptotic behavior is given by

$$\begin{array}{l} I_{s\nu lm} \rightarrow \psi_{s\nu}(i_s) P_{lm}(\Omega_s) v_s^{-\frac{1}{2}} r_s^{-1} \exp(-ik_s r_s), \\ E_{s\nu lm} \rightarrow \psi_{s\nu}(i_s) P_{lm}(\Omega_s) v_s^{-\frac{1}{2}} r_s^{-1} \exp(ik_s r_s). \end{array}$$

$$(30)$$

They are, of course, functions of the form (5).

The asymptotic form of the S and C is given by (26), the  $\mathfrak{D}$  and  $\mathfrak{V}$  are expressed in terms of

 $<sup>^{11}</sup>$  The following is the third property which was referred to in reference 4.

the S and C in (9), and the  $\varphi$  are expressed in terms of the D and U in (13). One obtains by means of these equations, for the  $\varphi$  in terms of the incoming and outgoing waves I and E,

$$\varphi_{sl\mu} = \frac{1}{2} \sum_{s'l'm} (\Re^{J} \Re \omega^{*} + i \Re)_{sl;s'l'}$$

$$\times s(j_{s'}, l')_{J\mu-mm} I_{s'\mu-ml'm}$$

$$+ \frac{1}{2} \sum_{s'l'm} (\Re^{J} \Re \omega - i \Re^{*})_{sl;s'l'}$$

$$\times s(j_{s'}, l')_{J\mu-mm} E_{s'\mu-ml'm}. \quad (31)$$

One can obtain from (31), by linear combination, a solution in which only one type of incident wave is present:

$$2 \sum_{s'l'} \{ (\Re^{J} \mathfrak{B} \omega^{*} + i \mathfrak{A})^{-1} \}_{sl; s'l'} \varphi_{s'l'\mu}$$
  
=  $\sum_{m} s(j_{s}, l)_{J\mu-mm} I_{s\mu-mlm}$   
-  $\sum_{s'l'm} u_{sl; s'l'} J_{s}(j_{s'}, l')_{J\mu-mm} E_{s'\mu-ml'm}, \quad (32)$ 

where

$$u_{sl;s'l'}{}^{J} = -\{(\Re^{J}\mathfrak{B}\omega^{*} + i\mathfrak{A})^{-1} \times (\Re^{J}\mathfrak{B}\omega - i\mathfrak{A}^{*})\}_{sl;s'l'}.$$
 (33)

From this, one obtains by means of the orthogonality relation of the coefficients s (Eq. (28), Chapter XVII of reference 6) a solution in which only one incident beam occurs. This becomes, in the external region,

$$I_{svlm} - \sum_{s'v'l'm'} U_{svlm; s'v'l'm'} E_{s'v'l'm'}, \quad (34)$$

in which

$$U_{s\nu lm; s'\nu' l'm'} = \sum_{J} s(j_{s}, l)_{J\nu m} u_{sl; s'l'}^{J} \times s(j_{s'}, l')_{J\nu'm'} \delta_{m+\nu, m'+\nu'}$$
(35)

is the ordinary collision matrix. The last factor of (35) expresses the conservation law for the Z component of the angular momentum since  $\nu$  is the Z component of the spins, and m is the Z component of the angular momentum of the relative motion of the two particles. The conservation law for the absolute value of the angular momentum is not immediately evident from the form (35) but is included in the s factors.

The symmetric and unitary nature of the  $\mathfrak{U}$  would follow at once from the orthogonality relations of the *s* coefficients if the symmetric unitary

nature of the  $\mathfrak{u}^J$  matrices were evident. If the spins of the particles are all zero, the  $\mathfrak{U}$  matrix in fact becomes, in the sense of reference 5, identical with  $\delta_{ll'}$  times the  $\mathfrak{u}^l$  matrix. It is desirable, for these reasons, to bring the  $\mathfrak{u}^J$  into a form in which their unitary and symmetric nature is at once apparent.

For this purpose we express  $\mathfrak{A}$  and  $\mathfrak{A}^*$ , by means of (29), in terms of the  $\mathfrak{B}$ ,  $\omega$ , and  $\mathfrak{C}$ :

$$\mathbf{\mathfrak{u}} = (\mathfrak{N}\mathfrak{B}\omega^* + \mathfrak{C}\mathfrak{B}^{-1}\omega^* + i\mathfrak{B}^{-1}\omega^*)^{-1} \times (-\mathfrak{N}\mathfrak{B}\omega - \mathfrak{C}\mathfrak{B}^{-1}\omega + i\mathfrak{B}^{-1}\omega).$$
(36)

The superscript J has been omitted on both sides. For the first factor one can write, since the  $\mathfrak{B}$ ,  $\omega$ ,  $\mathfrak{C}$  all commute,

$$[i\mathfrak{B}^{-1}(-i\mathfrak{B}\mathfrak{R}\mathfrak{B}-i\mathfrak{C}+1)\omega^*]^{-1} = -i\omega(1-i\mathfrak{B}\mathfrak{R}\mathfrak{B}-i\mathfrak{C})^{-1}\mathfrak{B}.$$
 (37)

The second factor can be transformed in a similar way to give  $i\mathfrak{B}^{-1}(i\mathfrak{B}\mathfrak{N}\mathfrak{B}+i\mathfrak{C}+1)\omega$ . Hence

$$\mathfrak{u}^{J} = \omega \frac{1 + i\mathfrak{B}\mathfrak{N}^{J}\mathfrak{B} + i\mathfrak{C}}{1 - i\mathfrak{B}\mathfrak{N}^{J}\mathfrak{B} - i\mathfrak{C}}.$$
(38)

It is permissible to use the fraction sign in (38) since both numerator and denominator depend on a single matrix:  $\mathfrak{W} \mathfrak{W} + \mathfrak{C}$ . Since this matrix is evidently symmetric and Hermitean, the fraction is symmetric and unitary and it remains such if multiplied both in front and in back by the unitary matrix  $\omega$ . Equations (35), (38), and (24) give the collision matrix in terms of real parameters. Although the values of these parameters are dependent on  $a_s$ , the collision matrix, which is a property of the physical system, must itself be independent of these quantities.

The wave function describing a collision experiment may be obtained by well-known procedures in terms of the collision matrix  $\mathfrak{ll}$ . The plane wave representing particles of type *s* moving along the *Z* axis has the form

$$iv_{s}^{-\frac{1}{2}}\exp(ik_{s}z_{s})\psi_{s\nu}(i_{s})$$

$$=\frac{\pi^{\frac{1}{2}}}{ik_{s}}\sum_{l}(2l+1)^{\frac{1}{2}}(E_{s\nu l0}-(-)^{l}I_{s\nu l0}).$$
(39)

This wave is normalized to unit current of the s particles per unit area normal to the beam. The normalization of the  $P_{10}$ , which are used in the

definition of E and I, is given by

$$P_{l0}(\Omega_s) = i((2l+1)/4\pi)^{\frac{1}{2}}P_l(\cos\theta_s),$$

where the  $P_l(\cos\theta_s)$  are the usual Legendre polynomials.

A continuable solution with the same incident waves as (39) may be formed by taking an appropriate linear combination of solutions of the type (34):

$$-\frac{\pi^{\frac{1}{2}}}{ik_{s}}\sum_{l}(-)^{l}(2l+1)^{\frac{1}{2}} \times \left(I_{s\nu l0}-\sum_{s'\nu'l'm'}U_{s\nu l0;s'\nu'l'm'}E_{s'\nu'l'm'}\right). \quad (40)$$

The continuable solution which satisfies the boundary conditions for an experiment involving collisions between the *s* particles, is obtained from (40) by adding and subtracting the emerging waves of (39). The wave function describing the collision system, therefore, is

$$iv_{s}^{-\frac{1}{2}}\exp(ik_{s}z_{s})\psi_{s\nu}(i_{s}) + \frac{\pi^{\frac{1}{2}}}{ik_{s}}\sum_{ls'\nu'l'm'} (2l+1)^{\frac{1}{2}} \times ((-)^{l}U_{s\nu l0;\ s'\nu'l'm'} - \delta_{s\nu l0;\ s'\nu'l'm})E_{s'\nu'l'm'}, \quad (41)$$
  
where

$$\delta_{s\nu l0}; \, {}_{s'\nu' l'm'} = \delta_{ss'} \delta_{\nu\nu'} \delta_{ll'} \delta_{0m'}.$$

The density of the s' systems resulting from the collision is obtained by squaring the part of the sum in (41) which refers to these systems and integrating over the internal coordinates  $i_{s'}$ . The number per second of s' systems crossing a surface subtending a solid angle  $d\Omega_{s'}$  at the collision center, is obtained from the density by multiplying with  $r_{s'}^2 v_{s'} d\Omega_{s'}$ . This is the differential cross section for the collision between the systems characterized by s with the polarization specified by  $j_s$  and  $\nu$ . The differential cross section is obtained by averaging the cross sections for all polarizations  $\nu$  and adding together the cross sections for all possible  $\nu'$ . This gives

$$d\sigma^{ss'} = \frac{\pi}{(2j_{s}+1)k_{s}^{2}} \sum_{\nu\nu'} \left| \sum_{ll'm'} (2l+1)^{\frac{1}{2}} \times \{(-)^{l} U_{s\nu l0; s'\nu' l'm'} - \delta_{s\nu l0; s'\nu' l'm'} \} \times P_{l'm'}(\Omega_{s'}) \right|^{2} d\Omega_{s'}, \quad (42)$$

for the differential cross section for the production of s' systems in a collision between unpolarized s systems. Integration of (42) over  $d\Omega_{s'}$  leads to the total cross section.

$$\sigma^{ss'} = \frac{\pi}{(2j_s+1)k_s^2} \sum_{\nu\nu'l'm'} \left| \sum_{l} (2l+1)^{\frac{1}{2}} \times \{(-)^l U_{s\nu l0; s'\nu'l'm'} - \delta_{s\nu l0; s'\nu'l'm'} \right|^2. \quad (43a)$$

If the  $\mathfrak{U}$  is replaced by the  $\mathfrak{U}^J$  by means of (35) this expression reduces, upon making use of the unitary character of the matrices formed by the s coefficients, to

$$\sigma^{ss'} = \frac{\pi}{(2j_s+1)k_s^2} \sum_{ll'J} \\ \times (2J+1) |(-)^l u_{sl;\ s'l'} - \delta_{sl;\ s'l'}|^2. \quad (43b)$$

One should remember when using the formulae (42), (43) that s (and s') specify not only the nature of the subsystems which react (and are formed by the reaction) but also their state of excitation and the resultant of their spin angular momentum  $j_s$  (and  $j_{s'}$ ). The cross section for the formation of a pair of nuclei without regard to the resultant  $j_{s'}$  of their spins is given by summing (42) and (43) over all s' which refer to the same pair of nuclei. Similarly, if one is interested in the cross section of a pair designated by s'without regard to  $j_s$ , one must average (42) and (43) over all s (which now refer to a definite pair of nuclei). This may be done by adding together the  $d\sigma^{ss'}$  or  $\sigma^{ss'}$  for the possible values of s with the statistical weights  $(2j_s+1)/\sum_{s} (2j_s+1)$ .

#### V. DISCUSSION: THE GENERALIZED ONE-LEVEL FORMULA

The results of the preceding sections have very great generality inasmuch as they permit one to express all scattering and reaction cross sections in terms of the energy-independent parameters  $E_{\lambda}$ ,  $\gamma_{\lambda sl}$ , etc. Their most unsatisfactory feature is that all these parameters depend on the arbitrary location of the boundary S of the internal region, i.e., on the constants  $a_s$ . Naturally the expressions (42) and (43) for the cross sections are independent of these quantities. It would be desirable to abstract from our representation of the

cross sections new concepts which have physical significance. Unfortunately,  $E_{\lambda}$  and  $\gamma_{\lambda sl}$ , since they depend on the  $a_s$ , cannot be given direct physical interpretation. Clearly, a close investigation of the dependence of the quantities  $E_{\lambda}$ ,  $\gamma_{\lambda sl}$  on the  $a_s$  is well warranted; such an investigation, however, has not yet been made.

Let us first choose the  $a_s$  as small as possible, i.e., choose an internal region which just barely satisfies the conditions enumerated in Section II. If we assume that  $|X_{\lambda\mu}|^2$  is just about as great on S as inside S, the integral of  $|X_{\lambda\mu}|^2$  over S will be of the order of magnitude of the reciprocal of the  $a_s$ . The integral of the  $|\mathcal{V}_{sl\mu}|^2$  over S is  $M_s/\hbar$ . As a result,  $\gamma_{\lambda sl}$ , the integral of the product of  $X_{\lambda\mu}^*\mathcal{V}_{sl\mu}$  over S, is by Schwartz's inequality limited by

$$\gamma_{\lambda s l} < \frac{\hbar}{(2M_s)^{\frac{1}{2}}} \left[ \int |X_{\lambda \mu}|^2 dS \right]^{\frac{1}{2}} \approx \frac{\hbar}{(M_s a_{\min})^{\frac{1}{2}}}, \quad (44)$$

where  $a_{\min}$  is a quantity of the order of the diameter of the compound nucleus. Actually the inequality sign in (44) is a very strong one and the comparison with observed neutron widths indicates<sup>12</sup> that the left side of (44) is usually a few thousand times smaller than the right side. (The relation between the  $\gamma_{\lambda sl}$  and the level width will be given later in this section.) This is not surprising considering that any similarity between the  $X_{\lambda\mu}$  and the  $\mathcal{U}_{sl\mu}$  would seem to be rather accidental. On the other hand, Eq. (44) suggests that the  $\gamma_{\lambda sl}$  should be of the same order of magnitude for different s and l.

We shall now assume that the interaction of the particles of the pair *s* has, in the external region, no term which goes to infinity for  $r_s \rightarrow 0$ except perhaps as  $Ze^2/r_s$ . If this is true, and if  $k_sr_s\ll 1$ , the  $\bigcup_{sl_{\mu}}$  defined in (9) will be proportional to  $r_s^{-l-1}$ , and the  $X_{\lambda\mu}$  will have the same behavior near the surface given by  $r_s = a_s$ . Hence,  $X_{\lambda\mu}$  which satisfies a boundary condition similar to (8) for a given  $a_s$ , will satisfy it also for another  $a_s$  as long as  $k_{\lambda s}a_s\ll 1$ . ( $k_s$  is the wave number of the separated pair *s* for the energy  $E = E_{\lambda}$ .) This shows that, as long as  $k_{\lambda s}a_s\ll 1$ , the  $E_{\lambda}$  are independent of the  $a_s$ . On the other hand, the  $\gamma_{\lambda s l}$  will depend on  $a_s$  like  $a_s^{-l}$ , because the  $X_{\lambda\mu}$  depends on  $r_s$  like  $r_s^{-l}$  in the neighborhood of  $r_s = a_s$ . As a result of this and (44), we can write

$$\gamma_{\lambda sl} = \theta_{\lambda sl} \hbar / (M_s a_{\min})^{\frac{1}{2}} (a_{\min}/a_s)^l, \qquad (45)$$

where  $\theta_{\lambda s l}$  is in many cases a number of the order of  $10^{-3}$ .

This last estimate of the  $\gamma$  will permit us to discuss the results of the preceding section under some simplifying assumptions. Since a complete discussion of those results would be tantamount to a discussion of scattering and reaction cross sections in general, this is all we can hope for at present.

For sake of simplicity, we shall consider only the  $\mathfrak{u}^J$  of (38). In principle, it should always be easy to obtain  $\mathfrak{U}$ , and hence also the cross sections, from  $\mathfrak{u}^J$  by means of (35). Thus,  $U_{s\nu lm; s'\nu' l'm'}$ is actually equal to  $u_{sl; s'\nu'}\delta_{ll\nu}\delta_{mm'}$ , if  $j_s = 0$ , i.e., if the spins of the colliding particles and of the reaction products both vanish (the  $\nu$  and  $\nu'$  as components of  $j_s$  and  $j_{s'}$  are also zero in this case).

The difficulty in obtaining  $\mathfrak{u}^J$  from  $\mathfrak{R}^J$  is one of matrix multiplication or division. As was pointed out in the last section of reference 1b, the matrix algebra can be carried out simply only if  $\mathfrak{R}$  is one or two dimensional, or if it is sufficient to restrict oneself to one or two terms in (24). These cases have been dealt with in reference 1b and will not be taken up again. We assume, instead, that one can replace all the terms of  $\mathfrak{R}$ , excepting one, by an energy-independent term:

$$\Re(E) = \frac{\gamma_{\lambda} \times \gamma_{\lambda}}{E_{\lambda} - E} + \Re_{\infty}.$$
 (46)

This  $\Re(E)$  has the same form which was obtained in reference 1a and consequently the following discussion shows a certain similarity with the one carried out there. In particular, it will lead to the generalized one-level formula obtained there, with the difference, however, that the orbital angular momenta of the particles will not be restricted to zero.

For convenience we introduce the abbreviations,  $\mathfrak{BR}_{\infty}\mathfrak{B} + \mathfrak{C} = \mathfrak{C}'$ , and  $\mathfrak{B}_{\Upsilon\lambda} = \mathfrak{g}_{\lambda}$ . Making use of the theorem  $\mathfrak{M}(\mathbf{y} \times \mathbf{y})\mathfrak{N} = (\mathfrak{M}\mathbf{y} \times \mathfrak{N}\mathbf{y})$ , if  $\mathbf{y}$  is an arbitrary vector and  $\mathfrak{N}$  a symmetric matrix we may write for (38)

$$\omega^{-1}\mathfrak{u}^{J}\omega^{-1} = \frac{1+i[(\mathfrak{g}_{\lambda}\times\mathfrak{g}_{\lambda})/(E_{\lambda}-E)]+i\mathfrak{C}'}{1-i[(\mathfrak{g}_{\lambda}\times\mathfrak{g}_{\lambda})/(E_{\lambda}-E)]-i\mathfrak{C}'}.$$
 (47)

<sup>&</sup>lt;sup>12</sup> L. J. Rainwater, W. W. Havens, C. S. Wu, and J. R. Dunning, Phys. Rev. **71**, 65 (1947); R. B. Sawyer, E. O. Wollan, K. C. Peterson, and S. Bernstein, Phys. Rev. **7.0** 791 (1946).

1	B <sub>sl</sub>	ω <sub>sl</sub>	C <sub>sl</sub>	$\Gamma_{\lambda sl}(\Re_{\infty}=0)$	$\Delta_{\lambda sl}(\Re_{\infty}=0)$
0	ks <sup>3</sup>	$\exp(-ix_s)$	0	$k_s \gamma_{\lambda s 0}^2$	0
1	ks <sup>3</sup>	$\exp(-ix_s)$	$-\frac{1}{x_s}$	$\frac{k_s x_s^2 \gamma_{\lambda s 1}^2}{1+{x_s}^2}$	$-\frac{k_s x_s \gamma_{\lambda s 1}^2}{1+{x_s}^2}$
2	$\frac{k_s^{\frac{1}{2}}}{x_s}(1+x_s^2)^{\frac{1}{2}}$	$-i\exp\{-i(x_s-\varphi_s)\}$ $(\varphi_s=\tan^{-1}x_s)$	$-\frac{1}{x_s^3}(3+2x_s^2)$	$\frac{k_s x_s^4 \gamma_{\lambda s 2}^{2} (1+x_s^2)}{(3+2x_s^2)^2+x_s^6}$	$-k_s x_s \gamma_{\lambda s 2}^2  imes rac{(1+x_s^2)(3+2x_s^2)}{(3+2x_s^2)^2+x_s^6}$

TABLE I. Coefficients in the cross-section formula (no interaction in the external region);  $x_s = k_s a_s$ .

We shall try to choose a parameter  $\eta$  so that the numerator of (47) may be written

$$1+i[(\mathfrak{g}_{\lambda}\times\mathfrak{g}_{\lambda})/(E_{\lambda}-E)]+i\mathfrak{G}'$$
  
=[1+i\mathfrak{G}'+i\eta(1-i\mathfrak{G}')^{-1}(\mathfrak{g}\_{\lambda}\times\mathfrak{g}\_{\lambda})]  
×[1-i(1-i\mathfrak{G}')^{-1}(\mathfrak{g}\_{\lambda}\times\mathfrak{g}\_{\lambda})/(E\_{\lambda}-E)]. (48)

Upon performing the multiplication and collecting terms, (48) reduces to

$$2(\mathfrak{g}_{\lambda} \times \mathfrak{g}_{\lambda}) = \eta [(E_{\lambda} - E)(\mathfrak{g}_{\lambda} \times \mathfrak{g}_{\lambda}) - i(\mathfrak{g}_{\lambda} \times \mathfrak{g}_{\lambda})(1 - i\mathfrak{G}')^{-1}(\mathfrak{g}_{\lambda} \times \mathfrak{g}_{\lambda})]. \quad (49)$$

If the elements of  $(\beta_{\lambda} \times \beta_{\lambda})(1-i\mathfrak{C}')^{-1}(\beta_{\lambda} \times \beta_{\lambda})$  are written in terms of the individual matrices involved it is seen that

$$(\mathbf{\mathfrak{g}}_{\lambda} \times \mathbf{\mathfrak{g}}_{\lambda})(1 - i \mathfrak{C}')^{-1}(\mathbf{\mathfrak{g}}_{\lambda} \times \mathbf{\mathfrak{g}}_{\lambda}) = \xi(\mathbf{\mathfrak{g}}_{\lambda} \times \mathbf{\mathfrak{g}}_{\lambda}), \quad (50)$$

where  $\xi$  is given by the scalar product

$$\xi = (\mathfrak{g}_{\lambda}, (1 - i\mathfrak{G}')^{-1}\mathfrak{g}_{\lambda}). \tag{51}$$

Introducing (50) into (49) we get

$$\eta = 2/(E_{\lambda} - E - i\xi). \tag{52}$$

If now we factor  $1-i\mathfrak{G}'$  out of the denominator of (47) so that both numerator and denominator have the common factor  $[1-i(1-i\mathfrak{G}')^{-1}(\mathfrak{g}_{\lambda}\times\mathfrak{g}_{\lambda})/(E_{\lambda}-E)]$ , we may replace (47) by

$$\omega^{-1}\mathfrak{u}^{J}\omega^{-1} = \frac{1+i\mathfrak{C}'}{1-i\mathfrak{C}'} + \frac{2i}{E_{\lambda}-E-i\xi} \times \{ [(1-i\mathfrak{C}')^{-1}\mathfrak{g}_{\lambda}] \times [(1-i\mathfrak{C}')^{-1}\mathfrak{g}_{\lambda}] \}.$$
(53)

(In writing the last matrix of (53) we have made use of the symmetry of  $(1-i\mathfrak{C}')^{-1}$  which follows from the symmetry of  $\mathfrak{C}'$ .) It is convenient to introduce a vector  $\alpha_{\lambda}$  defined by

$$\alpha_{\lambda} = (1 - i \mathfrak{C}')^{-1} \mathfrak{g}_{\lambda} = (1 - i \mathfrak{C}')^{-1} \mathfrak{B}_{\Upsilon \lambda}, \qquad (54)$$

so that

$$\beta_{\lambda} = (1 - i \mathfrak{C}') \alpha_{\lambda} = (1 + i \mathfrak{C}') \alpha_{\lambda}^{*}; \qquad (54a)$$

the last result follows from the reality of  $\beta_{\lambda}$ . By making use of (54) and (54a) we may divide  $\xi$  into its real and imaginary parts:

$$Re\xi = \frac{1}{2}\Gamma_{\lambda} = (\alpha_{\lambda}^{*}, \alpha_{\lambda}) = \sum_{sl} |\alpha_{\lambda sl}|^{2} = \frac{1}{2} \sum_{sl} \Gamma_{\lambda sl};$$
  
$$Im\xi = \Delta_{\lambda} = (\alpha_{\lambda}^{*}, \mathfrak{C}'\alpha_{\lambda})$$
(55)

 $\Gamma_{\lambda}$  will play the role of a level width: the  $2 |\alpha_{\lambda s l}|^2 = \Gamma_{\lambda s l}$  may be interpreted as the partial widths. As will be seen immediately, the  $\Delta_{\lambda}$  represents a shift in the position of the resonance from  $E_{\lambda}$ . With the help of (54) and (55) we may rewrite (53) as

$$\mathfrak{u}' = \omega \left(\frac{1+i\mathfrak{C}'}{1-i\mathfrak{C}'}\right) \omega + \frac{2i\omega(\alpha_{\lambda} \times \alpha_{\lambda})\omega}{E_{\lambda} + \Delta_{\lambda} - E - \frac{1}{2}i\Gamma_{\lambda}}.$$
 (56)

The total cross section (43b) may be obtained from the absolute squares of the elements of the matrix  $(-)^{i}\mathfrak{u}^{J}-1$ . The squares of the elements of the second matrix on the right of (56) represent the resonance part of the scattering or reaction. The elements of  $(-)^{i}\omega(1+i\mathfrak{C}')(1-i\mathfrak{C}')^{-1}\omega-1$ , which are slowly varying functions of the energy, give rise to what one may call "potential" scattering or reaction. The cross products represent the effects of interference between the resonance and potential terms. The potential term includes two contributions corresponding to the two terms of  $\mathfrak{C}'$ : the part which arises from  $\mathfrak{C}$  alone represents the scattering (since  $\mathfrak{C}$  is diagonal) of the incident particles which would be caused by the presence of an infinite positive potential within the internal region. The contribution of the  $\mathfrak{M}\mathfrak{M}_{\infty}\mathfrak{B}$  represents the effect of all levels other than the level  $E_{\lambda}$ . It will in general produce both scattering and reaction terms.

If  $\mathfrak{G}'$  is diagonal, the contribution to the total *reaction* cross section by the level  $E_{\lambda}$  is by (55), (56), and (43b)

$$\sigma^{ss'} = \frac{\pi}{(2j_s+1)k_s^2} \sum_{ll'} \frac{(2J+1)\Gamma_{\lambda sl}\Gamma_{\lambda s'l'}}{(E_\lambda + \Delta_\lambda - E)^2 + \frac{1}{4}\Gamma_\lambda^2}.$$
 (57)

Let us investigate now the dependence on  $a_s$ and energy of the different quantities which enter (56) and hence (57), at least in the case where the  $\Re_{\infty}$  of (46) can be neglected. We consider for simplicity the case of no interaction in the external region. The  $\mathcal{C}_{sl}$  and  $\mathcal{S}_{sl}$  which satisfy (8) are easily computed; comparison of the results with Eqs. (26) and (29) leads to the results of Table I. In computing this table we made use of the relations

$$\frac{1}{2}\Gamma_{\lambda sl} = (B_{sl}\gamma_{\lambda sl})^2/(1+C_{sl}^2), \qquad (58a)$$

$$\Delta_{\lambda} = \sum_{sl} \Delta_{\lambda sl}; \quad \Delta_{\lambda sl} = \frac{1}{2} C_{sl} \Gamma_{\lambda sl}, \qquad (58b)$$

$$\alpha_{\lambda sl} = (B_{sl}\gamma_{\lambda sl})^{-1}(\frac{1}{2}\Gamma_{\lambda sl} + i\Delta_{\lambda sl}), \qquad (58c)$$

which follow from (55) and (54) when  $\mathfrak{C}'$  is diagonal. The  $x_s$  in the table is an abbreviation for  $k_s a_s$ .

If the energy of the *s* systems is small and the  $a_s$  are taken small so that  $k_s a_s \ll 1$ , it is seen that the  $\Gamma_{\lambda sl}$  depend on energy as  $E^{(l+\frac{1}{2})}$ . Moreover, since  $\gamma_{\lambda sl}$  varies with  $a_s$  as  $a_s^{-l}$  (Eq. 45) it is seen that the  $\Gamma_{\lambda sl}$ , and hence the  $\Gamma_{\lambda}$  are approximately independent of  $a_s$  as long as  $a_s$  is small enough so that  $k_s a_s \ll 1$ . Under the conditions given, therefore, the  $\Gamma_{\lambda sl}$  have physical significance. It is to be noted also that because of (45), the partial widths for the higher orbital angular momenta are related to the partial widths for l=0, as far as order of magnitude is concerned, by

$$\Gamma_{\lambda s l} \approx x_s^{2l} \Gamma_{\lambda s 0}. \tag{59}$$

with

The  $\Delta_{\lambda}$  is roughly proportional to *E* if  $x_s$  is small. From (59) and (58b) it follows that the order of magnitude of the  $\Delta_{\lambda sl}$  is given by

$$\Delta_{\lambda sl} \sim -x_s \Gamma_{\lambda s0} (a_{\min}/a_s)^{2l}. \tag{60}$$

Thus the partial shifts are all very small and  $E_{\lambda}$  is practically independent of the  $a_s$ . As has already been mentioned, the fact that  $E_{\lambda}$  is essentially independent of  $a_s$  is a consequence of the boundary conditions which have been imposed on the  $X_{\lambda\mu}$  and  $C_{sl}$ .

For small  $k_s a_s$  the elements of the first matrix on the right of (56) are approximately

$$(-)^{l}$$
 + terms of order  $x^{2l+1}$ , (61)

from which it is seen that the contributions to the potential scattering, for small x, are small and that they decrease rapidly with increasing l.

The one-level formula which is essentially contained in Eq. (57), or in (56) and (43b), is only a rather special case of the general formula (38). If the approximation (46) is not permissible, (38)still contains a representation of the cross section even though it may not be possible to put it into so pragmatic a form as (57). Nevertheless, an evaluation of the cross section may still be possible in closed form, as evidenced e.g., in the twolevel formulae and the formulae for two alternative reactions, given in reference 1b. However, in such cases it may not always be possible to associate large values of the cross sections with energies in the neighborhood of  $E_{\lambda}$  or to predict even the qualitative behavior of the cross section as a function of energy from a knowledge of the  $\gamma_{\lambda}$ and  $E_{\lambda}$  alone.

As an example, we consider the collision of systems with zero spins between which there is no interaction whatever, so that the scattering cross section vanishes for all E. The wave function for the free particles with l=0 may be put in the form of (13) if we take

$$R = k^{-1} \tan ka. \tag{62}$$

This may be written as a series of partial fractions in conformity with (23):

$$R = \sum_{\lambda} \frac{\gamma_{\lambda}^2}{E_{\lambda} - E},\tag{63}$$

$$E_{\lambda} = \frac{\hbar^2}{2M} (2\lambda - 1)^2 \left(\frac{\pi}{2a}\right)^2;$$
  

$$\gamma_{\lambda} = (-)^{\lambda} \left(\frac{\hbar^2}{Ma}\right)^{\frac{1}{2}}.$$
(64)

Of course these equations follow also from the formalism of Section III. Substitution of  $\omega = \exp(-ika)$ ,  $B = k^{\frac{1}{2}}$ , C = 0, as given for the case of no interaction in the external region (Table I), and *R* from (62) into (38) leads to  $u^J = 1$ , i.e., to zero scattering cross section, as it must. However, this result appears as a cancellation of the effect of the resonance levels given in (64) with the effect of the deviation of  $\omega$  from 1. Obviously the knowledge of the  $E_{\lambda}$  and  $\gamma_{\lambda}$  alone is insufficient to provide us with a picture of the variation of the cross section with energy. In fact, if one tries, e.g., to estimate the scattering cross section at low energies by using for R the first term in its expansion (63) one obtains about  $0.1a^2$ . This result is not so bad if one has chosen a small value of a. However, if one chooses a large a, as one is entirely at liberty to do formally, this gives a grossly inaccurate picture of the cross section. Only by considering the effect of all levels on Rdoes one obtain the correct zero cross section.

This article is based on work performed under Contract No. w-35-058-eng-71 for the Manhattan Project at Clinton Laboratories.

PHYSICAL REVIEW

VOLUME 72, NUMBER 1

JULY 1, 1947

## Stress Relaxation across Grain Boundaries in Metals\*

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In order to elucidate further the concept of relaxation of shear stress across grain boundaries in metals, the temperature dependence of internal friction and rigidity modulus of 99.991 percent aluminum have been measured as a function of frequency of torsional vibration and as a function of grain size of the specimen. It has been found that for the same specimen, an increase of frequency of vibration shifts the internal friction curve and the rigidity relaxation curve ( $Q^{-1}$  and  $G/G_U$  versus temperature) to higher temperatures; and when the frequency of vibration is kept constant, a change in grain size of the specimen has

#### 1. INTRODUCTION

**I** T has been demonstrated<sup>1</sup> that the grain boundaries in metals behave in a viscous manner in the sense that they cannot sustain a shear stress. Thus, when an over-all stress, however small, is applied to a specimen, the shear stress across all grain boundaries will gradually relax. Because of this relaxation of shear stress, the stress no longer remains a unique function of the strain, and vice versa, in the conventionally elastic region, and this causes all kinds of anelastic effects. The locking effect of the grain edges and corners will insure that the over-all stress relaxation will be of limited extent for a fixed overall strain. The maximum amount of macroscopic shear stress relaxation in 99.991 percent polycrystalline aluminum (average grain diameter = 0.03 cm) determined by four independent types of anelastic-effect measurements (namely, internal friction, temperature variation of rigidity modulus, creep under constant stress and stress relaxation at constant strain) is 33 percent, which agrees fairly well with the theoretical value of 36 percent<sup>2</sup> calculated by assuming the grain boundaries to be viscous.

It has also been shown that the rate of the stress relaxation across grain boundaries is a function of the temperature of measurement and

<sup>\*</sup> This research was supported by ORI (Contract No. N6ori-20-IV). <sup>1</sup>T. S. Kê, Phys. Rev. **70**, 105(A) (1946); *ibid.*, **71**, 142(A) and 533 (1947).

the same effect as a change of the frequency of vibration The observed internal friction and rigidity relaxation can be expressed as functions of the parameter (G.S.) $\times f$  $\times \exp(H/RT)$ , where (G.S.) is the grain size or average grain diameter of the specimen, f is the frequency of vibration, and H is the heat of activation. It is shown that all these observed phenomena are necessary manifestations of the stress relaxation across grain boundaries arising from the viscous behavior of the grain boundaries in metals, which behavior has been demonstrated by previous anelastic-effect measurements.

<sup>&</sup>lt;sup>2</sup> C. Zener, Phys. Rev. 60, 906 (1941).