

## On the Mathematical Description of Light Nuclei by the Method of Resonating Group Structure

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The wave function for the composite nucleus is written as a properly antisymmetrized combination of partial wave functions, corresponding to various possible ways of distributing the neutrons and protons into various groups, such as alpha-particles, *di*-neutrons, etc. The dependence of the total wave function on the intergroup separations is determined by the variation principle. The analysis is carried out in detail for the case that the configurations considered contain only two groups. Integral equations are derived for the functions of separation. The associated Fredholm determinant completely determines the stable energy values of the system (Eq. (33)), Eq. (48) connects the asymptotic behavior of an arbitrary particular solution with that of solutions possessing a standard asymptotic form. With its help, the Fredholm determinant also determines all scattering and disintegration cross sections (Eqs. (50)···(54) and (57)), without the necessity of actually obtaining the intergroup wave functions. The expressions (43) and (60) obtained for the cross sections, taking account of spin effects, have general validity. Details of the application of the method of resonating group structure to actual problems are discussed.

### INTRODUCTION

#### Resonating group structure

A DESCRIPTION<sup>1</sup> of the nucleus which regards the neutrons and protons as spending part of their time in configurations corresponding, for example, to interacting alpha-particles, part of their time in other groupings, already takes into account to a large extent that intimate interaction between nuclear particles which is so entirely different from the situation in atomic structure, where the concept of average field is a reasonable approximation. In contrast to the Hartree-Fock procedure, the method of "resonating group structure" builds up a wave function for the whole nucleus out of partial wave functions which describe the close interaction within the individual groups. It is clear that in this way we take advantage from the beginning of the saturation character of nuclear binding, by which much the largest part of the energy of the compound nucleus is accounted for by the internal binding of the separate groups. On the other hand, the fact that the total wave function is built of a properly antisymmetrized combination of partial wave functions, corresponding to the various possible types of

groupings, shows that we are far from the picture which regards alpha-particles, for example, as having any real existence within the nucleus.

It is the purpose of this paper to derive the wave equation for resonating group structures and to show how the interaction integrals can be evaluated and how solutions can be obtained which give the positions of nuclear energy levels and the cross sections for scattering and disintegration. We start out by considering a system of  $m$  protons and  $n$  neutrons described by the  $m+n=N$  coordinates<sup>2a</sup>  $\mathbf{x}_1, \sigma_1; \mathbf{x}_2, \sigma_2; \dots; \mathbf{x}_m, \sigma_m; \mathbf{y}_1, \tau_1; \dots; \mathbf{y}_n, \tau_n$ , ( $\sigma$ 's are proton spins,  $\tau$ 's are neutron spins) which we may abbreviate as simply  $\mathbf{1}, \mathbf{2}, \dots, \mathbf{N}$ . In the approximation given by the method mentioned, the wave function  $\Psi$  of the whole system is written as the sum of parts, of which a given term represents the  $N$  particles sorted into groups in a particular way (configuration). Such a term is the product of wave functions  $\Phi$  describing the motion of the particles within each group, multiplied by a function  $F$  which depends on the positions,  $\mathbf{X}$ , and spin variables,  $m_s$ , of the different groups (the word spin referring here to the total internal

<sup>1</sup> Cf. preceding paper, where Appendix I gives an example which illustrates the following considerations. For a preliminary account of the present work, cf. Phys. Rev. **51**, 683 (1937).

<sup>2a</sup> In this paper, neutrons and protons are treated as different particles. Nothing essential is changed, however, if one uses the formalism of the isotopic spin variable and treats neutrons and protons as different states of one type of particle.

angular momentum of a group). The various unknown functions  $F^i$  belong to different configurations—thus, for  $\text{Li}^6$ ,  $F^1$  might represent the relative motion of a normal alpha-particle and a normal deuteron;  $F^2$  might similarly represent excited  $\text{Li}^5$  plus neutron, etc. The properly antisymmetrized wave function for the whole system has the form <sup>2b</sup>

$$\begin{aligned} \Psi(12 \cdots \mathbf{N}) &= (k_I^{1!} \cdots l_I^{1!} \cdots m!n!)^{-\frac{1}{2}} \\ &\times \sum_{\text{perm}} (\pm 1) \sum_{m^1} F^1(\mathbf{X}_I^1, m_I^1; \mathbf{X}_{II}^1, m_{II}^1; \cdots). \\ \Phi_I^1, m_I^1(1, 2, \cdots, \mathbf{k}_I^1; \mathbf{m}+1, \mathbf{m}+2, \cdots, \mathbf{m}+l_I^1) \\ &\times \Phi_{II}^1, m_{II}^1(\mathbf{k}_I^1+1, \cdots; \mathbf{m}+l_I^1+1, \cdots) \cdots \\ &+ (k_I^{2!} \cdots l_I^{2!} \cdots m!n!)^{-\frac{1}{2}} \sum_{\text{perm}} (\pm 1) \\ &\sum_{m^2} F^2(\mathbf{X}_I^2, m_I^2; \cdots) \Phi_{I, m_I^1}^2(1, 2, \cdots, \mathbf{k}_I^2; \cdots) \cdots \\ &\quad + \text{terms in } F^3, F^4, \cdots F^c. \quad (1) \end{aligned}$$

The symbol  $\sum_{\text{perm}} (\pm 1)$  indicates a summation running over all  $m!$  permutations of the protons and  $n!$  permutations of the neutrons, with a change in sign for odd permutations; the function  $\Psi$  as written is not normalized but the numerical factors simplify the normalization.<sup>3</sup> The  $\mathbf{X}$ 's are of the form

$$\mathbf{X}_I^1 = (\mathbf{x}_1 + \mathbf{x}_2 + \cdots + \mathbf{x}_{k_I} + \mathbf{y}_1 + \mathbf{y}_2 + \cdots + \mathbf{y}_{l_I}) / (k_I + l_I).$$

The subscript  $m_{II}$  on  $\Phi_{II}^1$  singles out that particular wave function for group  $II^1$  (possessing spin  $S_{II}^1$ ) which represents the  $z$  component of its angular momentum as having the value  $m_{II}^1$ ; the sum over the  $m$ 's is to give a partial wave function  $\Psi^1$  corresponding to definite values of the angular momentum of the whole system and its projection along the  $z$  axis (the same, of course, for all  $\Psi^i$ 's). Group I of configuration 1 is not in general the same as group I of configuration 2, etc. The  $\Phi$ 's, among which there are, for example, alpha-particle wave functions,

<sup>2b</sup> The following is simplified on first reading by supposing that the groups have no spin, as is the case for  $\alpha$ -particles.

<sup>3</sup> The terms of the first sum are identical in sets of  $u^1 = k_I^{1!} \cdots l_I^{1!} \cdots$  at a time because of the antisymmetry of the  $\Phi$ 's; there are  $v^1 = m!n! / k_I^{1!} \cdots l_I^{1!} \cdots$  different distributions of the neutrons and protons into the groupings  $I^1, II^1$ , etc.; if the different distributions were orthogonal, the normalizing factor for the first sum would be exactly  $(v^1)^{-\frac{1}{2}}(u^1)^{-1}$ .

are antisymmetric in neutrons and in protons.<sup>4</sup> Each  $\Phi$  is normalized, and the  $\Phi$ 's representing different states of the same group are orthogonal; thus,

$$\begin{aligned} \sum_{\sigma_1, \sigma_2, \tau_8, \tau_9} \int \Phi_{\alpha}^*(1, 2, 8, 9) \\ \times \Phi_{\beta}(1, 2, 8, 9) d\tau_{1, 2, 8, 9} = \delta_{\alpha\beta}, \quad (2) \end{aligned}$$

where by  $\int \cdots d\tau$  we mean here the integral with respect to any three independent variables, keeping the center of gravity fixed:

$$d\tau = d(\mathbf{x}_1, \mathbf{x}_2, \mathbf{y}_8, \mathbf{y}_9) / d\mathbf{X}_{1289}.$$

The  $\Phi$ 's may depend explicitly on the  $\mathbf{X}$ 's ("polarization").

#### Outline of procedure

The problem centers on the calculation of the functions  $F^i$ , which we determine uniquely by the condition that they shall give the best possible wave function of the form (1) in the sense of the variation principle:

$$\delta E = 0 \quad \left( E = \int \Psi^* H \Psi d\tau / \int \Psi^* \Psi d\tau \right). \quad (3)$$

Our program is as follows: We express (Eq. (13))  $\int \Psi^* H \Psi d\tau$  and  $\int \Psi^* \Psi d\tau$  in terms of the  $F^i$  and certain quantities representing the Hamiltonians of the individual configurations and the interactions responsible for the resonance of the nucleus between different configurations; then (specializing to the case of only two groups in each configuration) we vary  $E$  in (2) separately with respect to each of the  $c$  functions  $F^i$ , and obtain from the variation principle  $c$  simultaneous integro-differential equations ((17) and (25)) on the  $F^i$ ; through the use of a generalized Green's function we transform these equations to integral equations (Eq. (30)) of a well-known type; the condition that the Fredholm determinant of this set of equations shall vanish is found to determine energy levels, and also, phase shifts and transmutation probabilities, without calculation of the  $F^i$  themselves; finally, we go into some details of the numerical calculation of the Fredholm determinants encountered.

<sup>4</sup> When a group consists only of a single particle,  $\Phi$  is simply a  $\delta$  function.

INTEGRATION OVER INTERNAL DEGREES  
OF FREEDOM

**Normalization integral**

We have to express the integral  $\int \Psi^* \Psi d\tau$  and similar energy integrals in terms of the  $F$ 's. The contribution coming from  $\Psi^{i*} \Psi^j$  reduces to the integral of

$$\begin{aligned} & (k_{\text{I}}^i! k_{\text{II}}^i! \cdots l_{\text{I}}^i! \cdots k_{\text{I}}^j! k_{\text{II}}^j! \cdots l_{\text{I}}^j! \cdots)^{-\frac{1}{2}} \cdot \\ & \times \sum_{m^i} F^i(\mathbf{X}_{\text{I}}^i, m_{\text{I}}^i; \mathbf{X}_{\text{II}}^i, \cdots) \\ & \Phi^{i_{\text{ImI}}}(\mathbf{1}, \mathbf{2}, \cdots, \mathbf{k}_{\text{I}}^i; \mathbf{m}+1, \cdots, \mathbf{m}+1_{\text{I}}^i) \\ & \times \Phi^{i_{\text{IImII}}}(\mathbf{k}_{\text{I}}^i+1, \cdots, \mathbf{k}_{\text{I}}^i+\mathbf{k}_{\text{II}}^i; \mathbf{m}+1_{\text{I}}^i+1, \cdots) \cdots \\ & \sum_{\text{perm}} (\pm 1) \sum_{m^j} F^j(\mathbf{X}_{\text{I}}^j, \cdots) \Phi^{j_{\text{ImI}}}(\mathbf{1}, \cdots, \mathbf{k}_{\text{I}}^j; \cdots) \cdots \quad (4) \end{aligned}$$

owing to the complete antisymmetry of the individual configuration wave functions  $\Psi^i$ . Imagine  $a_{\text{I I}}$  protons to be withdrawn from the  $k_{\text{I}}^i$  in group I of configuration  $i$  and placed in the group I of configuration  $j$ ,  $a_{\text{I II}}$  to be removed from the same source to II $^j$ , and so on; similarly we transfer  $b_{\text{I I}}$  neutrons from I $^i$  to I $^j$ , etc. Then the set of numbers  $a_{rs}$ ,  $b_{tu}$  describes a certain shifting of particles which may call the *linkage*  $\{ab\}$  from configuration  $i$  to  $j$ . Clearly

$$\begin{aligned} \sum_s a_{rs} &= k_r^i; & \sum_r a_{rs} &= k_s^j; \\ \sum_u b_{tu} &= l_t^i; & \sum_t b_{tu} &= l_u^j. \end{aligned}$$

(In the example following Eq. (26), for  $i=1$ ,  $j=2$ , we have  $a_{\text{I I}}=a_{\text{II I}}=b_{\text{I I}}=b_{\text{II I}}=0$ ,  $a_{\text{I II}}=a_{\text{II II}}=b_{\text{II I}}=b_{\text{II II}}=1$ ).

All  $a_{\text{I I}}! a_{\text{II I}}! \cdots b_{\text{I I}}! b_{\text{II I}}! \cdots$  terms in  $\sum_{\text{perm}}$  which belong to the same linkage are identical; terms belonging to a different set of values of the  $a$ 's and  $b$ 's are different from these [unless there are two or more group wave functions among either the  $\Phi^{i_{\text{ImI}}}$ ,  $\Phi^{i_{\text{IImII}}}$ ,  $\cdots$  or the  $\Phi^{j_{\text{ImI}}}$ ,  $\Phi^{j_{\text{IImII}}}$ ,  $\cdots$ , which are actually the same. When this situation occurs, the same linkage will be said to include those sets of values of the  $a_{rs}$ ,  $b_{tu}$  which arise by permuting the subscripts of identical states of individual groups in configuration  $i$  and by changing about the labels I, II,  $\cdots$  of those states  $\Phi^{i_{\text{ImI}}}$ ,  $\Phi^{i_{\text{IImII}}}$ ,  $\cdots$  which are really the same. If  $\lambda^i$  and  $\lambda^j$  are, respectively, the numbers of such per-

mutations, which do not actually have any effect on the distribution of particles into groups, then we introduce  $1/\lambda^i$  and  $1/\lambda^j$  as additional normalizing factors for the parts  $\Psi^i$  and  $\Psi^j$  of  $\Psi$  Eq. (1). Then the procedure goes through exactly as below, where we explicitly assume that all groups are different, so as to avoid unessential complications]. By defining numerical factors

$$g^{\{ab\}} = \frac{a_{\text{I I}}! a_{\text{II I}}! \cdots b_{\text{I I}}! \cdots}{[k_{\text{I}}^i! \cdots l_{\text{I}}^i! \cdots k_{\text{I}}^j! \cdots]^{\frac{1}{2}}},$$

we conveniently combine all terms belonging to the same linkage:

$$\begin{aligned} \int \Psi^* \Psi d\tau &= \sum_{i,j} \sum_{m^i, m^j} \sum_{\{ab\}_{ij}} g^{\{ab\}_{ij}} \\ & \times \int F^{i*}(\mathbf{X}_{\text{I}}^i, m_{\text{I}}^i, \cdots) \Phi^{i_{\text{ImI}}}(\mathbf{1}, \mathbf{2}, \cdots) \cdots \\ & \times F^j(\mathbf{X}_{\text{I}}^j, \cdots) \Phi^{j_{\text{ImI}}}(\cdots) \cdots d\tau. \quad (5) \end{aligned}$$

When in (5)  $\{ab\}_{ij}$  is the identical linkage ( $a_{\text{I I}}=k_{\text{I}}$ ,  $a_{\text{I II}}=0$ , etc.), then the normalization and orthogonality of the  $\Phi$ 's reduces the corresponding terms in the sum to

$$\begin{aligned} & \delta_{ij} \sum_{m^i} \int F^{i*}(\mathbf{X}_{\text{I}}^i, m_{\text{I}}^i, \cdots) F^i(\mathbf{X}_{\text{I}}^i, m_{\text{I}}^i, \cdots) \\ & \times d(\mathbf{X}_{\text{I}}^i, \cdots) / d\mathbf{A}, \quad (6) \end{aligned}$$

where  $\mathbf{A}$  represents the (vector) coordinate of the center of gravity and we have used the identity

$$\begin{aligned} & \frac{d(\mathbf{1}, \cdots, \mathbf{k}_{\text{I}}^i; \mathbf{m}, \cdots)}{d\mathbf{X}_{\text{I}}^i} \frac{d(\mathbf{k}_{\text{I}}^i+1, \cdots)}{d\mathbf{X}_{\text{II}}^i} \cdots \\ & \times \frac{d(\mathbf{X}_{\text{I}}^i, \mathbf{X}_{\text{II}}^i, \cdots)}{d\mathbf{A}} = \frac{d(\mathbf{1}, \cdots, \mathbf{N})}{d\mathbf{A}}. \end{aligned}$$

(In general,  $\frac{d\{f_1(xyz), f_2(xyz), f_4(xyz)\}}{dx}$  is defined

$$\text{to be } \frac{\partial(f_1, f_2, f_3)}{\partial(x, y, z)} dydz.)$$

For all other linkages in the sum (5), the  $\mathbf{X}^i$ 's, regarded as functions of the neutron and proton coordinates, will not all be the same as the  $\mathbf{X}^j$ 's. As it is complicated to carry out the treatment

from this stage on in detail in the general case, we specialize now to the case that there are only two groups in each of the  $c$  configurations. Then when  $\{ab\}$  is not the identical linkage, clearly the vectors  $\mathbf{X}_{\text{II}}^i - \mathbf{X}_{\text{I}}^i = \mathbf{X}_{\{ab\}}$  and  $\mathbf{X}_{\text{II}}^j - \mathbf{X}_{\text{I}}^j = \boldsymbol{\xi}_{\{ab\}}$  are independent of each other. We can therefore express the coordinates  $\mathbf{x}_1, \dots, \mathbf{x}_m, \mathbf{y}_1, \dots, \mathbf{y}_n$  in terms of  $\mathbf{A}, \mathbf{X}_{\{ab\}}, \boldsymbol{\xi}_{\{ab\}}$ , and  $N-3$  independent (vector) variables  $\mathbf{u}_4, \dots, \mathbf{u}_N$  by a linear substitution. The differential element  $d\tau$  becomes

$$d\tau = \frac{\partial(1, \dots, N)}{\partial(\mathbf{A}, \mathbf{X}, \boldsymbol{\xi}, \mathbf{u}_4, \dots, \mathbf{u}_N)} d\mathbf{X} d\boldsymbol{\xi} d\mathbf{u}_4 \dots d\mathbf{u}_N.$$

Since the  $\mathbf{u}$ 's do not enter in the  $F$ 's, and moreover we take the  $F$ 's to be independent<sup>5</sup> of  $\mathbf{A}$ , it follows that the integral in which we are interested reduces after integration over the  $\mathbf{u}$ 's to the form

$$\sum_{m^i, m^j} \sum_{\{ab\}_{ij}} \int \int F_i^*(\mathbf{X}_{\{ab\}_{ij}}; m_{\text{I}}^i, m_{\text{II}}^i) \times \mathbf{I}_{\{ab\}_{ij}}(\mathbf{X}_{\{ab\}}, m_{\text{I}}^i, m_{\text{II}}^i; \boldsymbol{\xi}_{\{ab\}}, m_{\text{I}}^j, m_{\text{II}}^j) \times F_j(\boldsymbol{\xi}_{\{ab\}}; m_{\text{I}}^j, m_{\text{II}}^j) d\mathbf{X}_{\{ab\}} d\boldsymbol{\xi}_{\{ab\}}. \quad (7)$$

We regard the functions  $F^i(\mathbf{X}, m_{\text{I}}, m_{\text{II}})$  which are obtained when the two  $m$ 's run over their allowed values ( $m_{\text{I}}^i = -S_{\text{I}}^i, \dots, S_{\text{I}}^i - 1, S_{\text{I}}^i$ ; etc.) as components of a single spin vector  $\mathbf{F}_i(\mathbf{X})$ , and similarly consider the quantities  $\mathbf{I}$  in Eq. (7) as components of a spin matrix  $\mathbf{I}_{\{ab\}_{ij}}(\mathbf{X}, \boldsymbol{\xi})$ . The  $\mathbf{X}$ 's and  $\boldsymbol{\xi}$ 's in the sum of integrals in Eq. (7) are dummy variables in the sense that they drop out of the integrated answer. Consequently, in spite of their different physical origin, we sum the spin matrices  $\mathbf{I}_{\{ab\}_{ij}}$  over all the different linkages joining the given configurations  $i$  and  $j$  (except the identical linkage), and denote the result as  $\mathbf{I}_{ij}(\mathbf{X}, \boldsymbol{\xi})$  ("overlapping integral"). On using a dot to indicate the inner product of spin vectors, we have finally

$$\int \Psi^* \Psi d\tau = \sum_{i=1}^c \int \mathbf{F}_i^*(\mathbf{X}) \cdot \mathbf{F}_i(\mathbf{X}) d\mathbf{X} + \sum_{i,j}^c \int \int \mathbf{F}_i^*(\mathbf{X}) \cdot \mathbf{I}_{ij}(\mathbf{X}, \boldsymbol{\xi}) \cdot \mathbf{F}_j(\boldsymbol{\xi}) d\mathbf{X} d\boldsymbol{\xi}, \quad (8)$$

<sup>5</sup> It being most convenient to calculate cross sections in the frame of reference in which the center of gravity is at rest:  $\mathbf{P} = \mathbf{O}$  in the factor  $\exp(i\mathbf{P}\mathbf{A}/\hbar)$  of  $F$ .

where the  $\mathbf{I}$ 's are in principle known functions of  $\mathbf{X}$  and  $\boldsymbol{\xi}$ , the form of the dependence being determined by the nature of the group wave functions  $\Phi$ .

### Kinetic and potential energy integrals

The calculation of the kinetic energy follows the preceding division into the cases of identical and nonidentical linkages. In the first case we express the  $k_{\text{I}}$   $\mathbf{x}$ 's and  $l_{\text{I}}$   $\mathbf{y}$ 's of the particles of the first group in terms of  $\mathbf{A}, \mathbf{X}$  and additional variables  $\mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_{k_{\text{I}}+l_{\text{I}}}$  by a linear orthogonal substitution, and similarly put in the coordinates of the particles of the second group as functions of  $\mathbf{A}, \mathbf{X}, \mathbf{w}_2, \mathbf{w}_3, \dots, \mathbf{w}_{k_{\text{II}}+l_{\text{II}}}$ . Then

$$\frac{\partial}{\partial \mathbf{x}_1} = \frac{1}{N} \frac{\partial}{\partial \mathbf{A}} - \frac{1}{k_{\text{I}}+l_{\text{I}}} \frac{\partial}{\partial \mathbf{X}} + \frac{\partial \mathbf{v}_2}{\partial \mathbf{x}_1} \frac{\partial}{\partial \mathbf{v}_2} + \dots,$$

and the kinetic energy operator becomes

$$T = (\hbar^2/2M) \{ N^{-1} \nabla_{\mathbf{A}} \cdot \nabla_{\mathbf{A}} + [(k_{\text{I}}+l_{\text{I}})^{-1} + (k_{\text{II}}+l_{\text{II}})^{-1}] \nabla_{\mathbf{X}} \cdot \nabla_{\mathbf{X}} + \sum_{\alpha} c_{\alpha} \nabla_{\mathbf{v}_{\alpha}} \cdot \nabla_{\mathbf{v}_{\alpha}} + \sum_{\alpha} d_{\alpha} \nabla_{\mathbf{w}_{\alpha}} \cdot \nabla_{\mathbf{w}_{\alpha}} \}, \quad (9)$$

where the  $c_{\alpha}$  and  $d_{\alpha}$  are numbers depending on the choice of the  $\mathbf{v}$ 's and  $\mathbf{w}$ 's and the first and second gradients in each pair act on  $\mathbf{F}_i^*(\mathbf{X}) \Phi_{\text{I}}^{i*} \Phi_{\text{II}}^{i*}$  and  $\mathbf{F}_j(\mathbf{X}) \Phi_{\text{I}}^j \Phi_{\text{II}}^j$ , respectively. In terms of the reduced mass  $\mu_i = \mu_j$  of the two groups, the kinetic energy integral for the identical linkage reduces to an expression of the form

$$\delta_{ij} (\hbar^2/2\mu_i) \int \nabla_{\mathbf{X}} \mathbf{F}_i^*(\mathbf{X}) \cdot \nabla_{\mathbf{X}} \mathbf{F}_i(\mathbf{X}) d\mathbf{X} + \int \mathbf{F}_i^*(\mathbf{X}) \cdot \mathbf{T}_{ij}(\mathbf{X}) \mathbf{F}_j(\mathbf{X}) d\mathbf{X}, \quad (10)$$

provided either that we do not allow the  $\Phi$ 's to depend on  $\mathbf{X}$  (no explicit polarization effects) or that we do not have in  $\Psi$  any configurations differing only by the internal state of excitation of the individual groups. [In the latter case, where the  $\Phi$ 's may involve  $\mathbf{X}$  as well as the  $\mathbf{u}$ 's and  $\mathbf{v}$ 's, we arrange that no terms occur in (10) which arise from derivatives of the type  $(\nabla_{\mathbf{X}} \mathbf{F}^*) \cdot \mathcal{I} \Phi_{\text{I}}^{i*} (\nabla_{\mathbf{X}} \Phi_{\text{I}}^j) d\mathbf{v} \mathbf{F}$ , by suitably choosing the arbitrary multiplicative functions  $\exp$  (if  $\mathbf{X}$ ) left free by the normalization and orthogonality conditions on the  $\Phi$ 's. There will however be

terms typified by  $\nabla_X \Phi_I^{i*} \cdot \nabla_X \Phi_I^i$ , which are included in  $\mathbf{T}_{ij}(\mathbf{X})$  along with the contributions of the proper internal kinetic energy operator ( $\hbar^2/2M \sum_{\alpha} c_{\alpha} \nabla_{v_{\alpha}} \cdot \nabla_{v_{\alpha}}$  of group I.) It is quite natural that there should be this exclusive relation between treatment by excited states and by explicit polarization of the groups, for the two are to a large extent equivalent methods of describing the same phenomenon.

Kinetic energy terms belonging to nonidentical linkages are reducible to expressions containing the  $F$ 's alone by use of the variables  $\mathbf{A}$ ,  $\mathbf{X}_{\{ab\}}$ ,  $\xi_{\{ab\}}$ ,  $\mathbf{u}_a, \dots, \mathbf{u}_N$  introduced above. The transformation is not in general orthogonal and consequently the kinetic energy operator (center of gravity at rest) becomes the linear combination of operators of the form

$$\nabla_X \cdot \nabla_X, \quad \nabla_X \cdot \nabla_{\xi}, \quad \nabla_X \cdot \nabla_{u_{\alpha}}, \quad \nabla_{u_{\alpha}} \cdot \nabla_{u_{\beta}}.$$

The first gradient in each pair acts on  $\mathbf{F}_i^*(\mathbf{X}) \Phi_I^{i*} \Phi_{II}^{i*}$ , the second on  $\mathbf{F}_j(\xi) \Phi_I^j \Phi_{II}^j$ . From  $\nabla_X \cdot \nabla_X$  originate the terms

$$[\nabla_X \mathbf{F}_i^*(\mathbf{X})] \Phi_I^i \Phi_{II}^i \mathbf{F}_j(\xi) [\nabla_X \Phi_I^j \Phi_{II}^j]$$

and  $\mathbf{F}_i(\mathbf{X}) [\nabla_X \Phi_I^i \Phi_{II}^i] \mathbf{F}_j(\xi) [\nabla_X \Phi_I^j \Phi_{II}^j]$ .

By partial integration of the first term with respect to  $\mathbf{X}$ , and use of the boundary condition<sup>6</sup> that  $\mathbf{F}_i(\mathbf{X})$  must vanish at infinity, we transform the first term to one where  $\mathbf{F}_i$  and  $\mathbf{F}_j$  appear undifferentiated. Continuing in this way with all the operators above, and then introducing new variables  $\mathbf{X}$ ,  $\xi$ ,  $\mathbf{u}$  to treat the next linkage, etc., we obtain finally the kinetic energy integral for all nonidentical linkages in the form

$$\sum_{i,j} \int \mathbf{F}_i^*(\mathbf{X}) \cdot \mathbf{T}_{ij}(\mathbf{X}, \xi) \cdot \mathbf{F}_j(\xi) d\mathbf{X} d\xi. \quad (11)$$

The remaining terms in the integral  $\int \Psi^* H \Psi d\tau$  come from the potential energy. If the forces between the elementary particles were ordinary interactions, the above analysis of the linkages would be valid, but the presence of exchange potentials will change some of the identical

<sup>6</sup> Only in the derivation do we make this restriction, which would, for the continuous spectrum, require us to deal always with a finite if small energy spread in the wave-function (which is of course physically correct), but in the actual calculations with the integro-differential equation below it is permissible to deal in the usual way with sharp energy values and waves which extend to infinity.

linkages to nonidentical linkages, and *vice versa*. Nevertheless, for each term there will be a suitable transformation of variables, either of the type  $\mathbf{A}$ ,  $\mathbf{X}$ ,  $\mathbf{v}$ ,  $\mathbf{w}$  or of the type  $\mathbf{A}$ ,  $\mathbf{X}$ ,  $\xi$ ,  $\mathbf{u}$ , which will finally reduce the total potential energy to the form

$$\sum_{i,j} \int \mathbf{F}_i^*(\mathbf{X}) \cdot \mathbf{U}_{ij}(\mathbf{X}) \cdot \mathbf{F}_j(\mathbf{X}) d\mathbf{X} + \sum_{i,j} \int \int \mathbf{F}_i^*(\mathbf{X}) \cdot \mathbf{U}_{ij}(\mathbf{X}, \xi) \cdot \mathbf{F}_j(\xi) d\mathbf{X} d\xi, \quad (12)$$

regardless of the type of the forces.<sup>7</sup>

For large values of  $\mathbf{X}$  and  $\xi$ , it follows from the finite extension of the individual group wave functions  $\Phi$  that the  $\mathbf{U}_{ij}(\mathbf{X}, \xi)$  and  $\mathbf{T}_{ij}(\mathbf{X}, \xi)$  tend to zero. At the same time, owing to the normalization and orthogonality of the  $\Phi$ 's,  $\mathbf{U}_{ij}(\mathbf{X}) + \mathbf{T}_{ij}(\mathbf{X})$  approaches  $\delta_{ij}$  times  $E_i$ , the energy attributable to the internal binding of the separated groups of configuration  $i$ . We therefore write  $\mathbf{U}_{ij}(\mathbf{X}) + \mathbf{T}_{ij}(\mathbf{X}) = E_i \delta_{ij} + V_{ij}(\mathbf{X})$  and also combine the interchange integrals:

$$\mathbf{U}_{ij}(\mathbf{X}, \xi) + \mathbf{T}_{ij}(\mathbf{X}, \xi) = \mathbf{J}_{ij}(\mathbf{X}, \xi).$$

Summarizing the above considerations, we find that in the approximation given by the method of resonating group structure, the energy of the compound system is

$$E = N/D,$$

where

$$\begin{aligned} N = & \sum_i (\hbar^2/2\mu_i) \int \nabla_X \mathbf{F}_i^*(\mathbf{X}) \cdot \nabla_X \mathbf{F}_i(\mathbf{X}) d\mathbf{X} \\ & + \sum_i E_i \int \mathbf{F}_i^*(\mathbf{X}) \cdot \mathbf{F}_i(\mathbf{X}) d\mathbf{X} \\ & + \sum_{i,j} \int \mathbf{F}_i^*(\mathbf{X}) \cdot \mathbf{V}_{ij}(\mathbf{X}) \cdot \mathbf{F}_j(\mathbf{X}) d\mathbf{X} \\ & + \sum_{i,j} \int \int \mathbf{F}_i^*(\mathbf{X}) \cdot \mathbf{J}_{ij}(\mathbf{X}, \xi) \cdot \mathbf{F}_j(\xi) d\mathbf{X} d\xi, \end{aligned}$$

and

$$\begin{aligned} D = & \sum_i \int \mathbf{F}_i^*(\mathbf{X}) \cdot \mathbf{F}_i(\mathbf{X}) d\mathbf{X} + \sum_{i,j} \int \int \mathbf{F}_i^*(\mathbf{X}) \\ & \cdot \mathbf{I}_{ij}(\mathbf{X}, \xi) \cdot \mathbf{F}_j(\xi) d\mathbf{X} d\xi. \quad (13) \end{aligned}$$

<sup>7</sup> They may be many-body interactions, for example.

## THE WAVE EQUATION

## Application of variation principle

It is known<sup>8</sup> that the Schroedinger wave equation may be derived from the variation principle  $\delta E=0$ , and that any improvement in an approximate wave function lowers the corresponding value of the energy.

We therefore determine the unknown functions  $\mathbf{F}$  by the condition that they shall give the best possible total wave function  $\Psi$  of the form (1) in the sense of the variation principle

$$\delta E = \delta(N/D) = 0. \quad (14)$$

The variation in  $N$  caused by a change  $\delta\mathbf{F}_i \delta(\mathbf{X}-\mathbf{X}_0)$  in the value of  $\mathbf{F}_i(\mathbf{X})$  at the point  $\mathbf{X}_0$  is found by partial integration to be<sup>9</sup>  $2\delta\mathbf{F}_i$  times

$$-(\hbar^2/2\mu_i)\nabla_{\mathbf{X}}^2\mathbf{F}_i(\mathbf{X}) + E_i\mathbf{F}_i(\mathbf{X}) + \sum_j \mathbf{V}_{ij}(\mathbf{X}) \cdot \mathbf{F}_j(\mathbf{X}) + \sum_j \int \mathbf{J}_{ij}(\mathbf{X}, \xi) \cdot \mathbf{F}_j(\xi) d\xi \quad (15)$$

evaluated at  $\mathbf{X}=\mathbf{X}_0$ . Similarly, the change in  $D$  is  $2\delta\mathbf{F}_i$  times

$$\mathbf{F}_i(\mathbf{X}) + \sum_j \int \mathbf{I}_{ij}(\mathbf{X}, \xi) \cdot \mathbf{F}_j(\xi) d\xi. \quad (16)$$

$E$  is stationary with respect to all variations of the  $\mathbf{F}$ 's only if the ratio  $\delta N/\delta D$  is the same as  $N/D=E$  for all values of  $\mathbf{X}_0$  and all values of  $i$ , whence we have the system of simultaneous linear integro-differential equations

$$\begin{aligned} & [(\hbar^2/2\mu_i)\nabla_{\mathbf{X}}^2 + E - E_i]\mathbf{F}_i(\mathbf{X}) \\ &= \sum_j \left[ \mathbf{V}_{ij}(\mathbf{X}) \cdot \mathbf{F}_j(\mathbf{X}) + \int \{ \mathbf{J}_{ij}(\mathbf{X}, \xi) - E\mathbf{I}_{ij}(\mathbf{X}, \xi) \} \right. \\ & \quad \left. \cdot \mathbf{F}_j(\xi) d\xi \right]. \quad (17) \end{aligned}$$

If the right member of (17) were zero, the solution of our equations would give simply the free relative motion of the different groups of a given configuration; the terms with  $j=i$  on the right

<sup>8</sup> E. Schroedinger, *Ann. d. Physik* 79, 362 (1926); cf. also R. Courant and D. Hilbert, *Methoden der Mathematischen Physik I*, second edition (Berlin, 1931), p. 159.

<sup>9</sup> We carry out the derivation as if the  $\mathbf{F}$ 's,  $\mathbf{V}$ 's,  $\mathbf{J}$ 's, and  $\mathbf{I}$ 's were all real; the result is however true in general. Cf. W. Heisenberg, *The Physical Principles of the Quantum Theory* (Chicago, 1930), p. 163.

determine the interaction between these groups, and the nondiagonal terms take into account the resonance between different configurations—in particular, the possibility of transmutations. From the fact that the energy of the system is always real we have<sup>10</sup>

$$\begin{aligned} \mathbf{V}_{ij}(\mathbf{X}) &= \mathbf{V}_{ji}^*(\mathbf{X}), \quad \mathbf{J}_{ij}(\mathbf{X}, \xi) = \mathbf{J}_{ji}^*(\xi, \mathbf{X}), \\ \mathbf{I}_{ij}(\mathbf{X}, \xi) &= \mathbf{I}_{ji}^*(\xi, \mathbf{X}). \end{aligned} \quad (18)$$

## Angular dependence

Owing to the intimate interaction which occurs in the compound nucleus, neither the internal angular momenta of the groups nor their mutual angular momentum  $L$  will be constant, but only the total angular momentum  $J$  and its projection  $m_J$  along a fixed space axis. We build up an eigenstate for a given  $J$  and  $m_J$  in two steps:  $S_I, S_{II} \rightarrow S; S, L \rightarrow J$ . To form a wave function corresponding to a particular value of the total internal group angular momentum,  $S$ , we have to take a definite<sup>11</sup> linear combination of the sets of states belonging to  $S_I$  and  $S_{II}$ :

$$\Phi^{i_s, m_s} = \sum_{m_I(m_{II})} \{ S^i, S_I^i, S_{II}^i; m_s, m_I, m_{II} \} \times \Phi^{i_s, m_I} \Phi^{i_{II}, m_{II}}. \quad (19)$$

The coefficients  $\{ \}$  are pure numbers; they vanish unless  $m_{II} = m_s - m_I$ , for which reason  $m_{II}$  is put in parenthesis in the sum.

We combine the  $\Phi$ 's for a given  $S$  with functions belonging to a definite state of relative angular momentum  $L$  (and projection  $m$ ) of the two groups and express the separation vector  $X$  in polar coordinates  $r, \theta, \varphi$ . The function

$$(1/r)f_J(i, L, S, r) \sum_{m(m_s)} \{ JLS; m_J m m_s \} \times Y_L^{(m)}(\theta, \varphi) \Phi^{i_s m_s} \quad (20)$$

belongs to a given value of the total angular momentum  $J$  and its projection  $m_J$ , and  $\mathbf{F}_i(\mathbf{X})\Phi_I^i\Phi_{II}^i$  will be made up of the sum of such functions over all values of  $L$  and  $S$  which are

<sup>10</sup> The star of a spin matrix indicates here its conjugate transposed.

<sup>11</sup> Cf. E. Wigner, *Gruppentheorie*, Eqs. (18a) and (27). (Braunschweig, 1931), p. 206. It is supposed that the normalizing constants in the  $\Phi$ 's are chosen with the proper sign. Three choices of sign for the related spherical harmonics  $Y_L^{(m)}$  are given in the literature; for that consistent with (19), and for tables of the  $\{ \}$ , cf. Condon and Shortley, *The Theory of Atomic Spectra* (Cambridge, 1935), p. 52, p. 75.

consistent with  $S_I$ ,  $S_{II}$ , and  $J$  according to the vector rule of addition of angular momenta. Consequently, for the given  $J$  and  $m_J$ , the  $m_I$ ,  $m_{II}$  component of the spin vector  $\mathbf{F}_i$  is

$$F^i(\mathbf{X}, m_I, m_{II}) = \sum_{\substack{L, S \\ (m), (m_S)}} (1/r) f_J(iLSr) \\ \times \{JLS; m_J m m_S\} Y_L^{(m)}(\theta, \varphi) \\ \times \{SS_I S_{II}; m_S, m_I, m_{II}\} \quad (21)$$

with suitably chosen  $f_J$ .

Clearly the left member of the  $i$ th integro-differential Eq. (17) will have the same form as (21) except that the  $f_J(iLSr)$  will appear operated on by

$$(1/r) [(\hbar^2/2\mu_i)((d^2/dr^2) - L(L+1)/r^2) \\ + E - E_i]. \quad (22)$$

We now multiply this number by  $r Y_L^{(m)*}(\theta, \varphi) \times \sin \theta d\theta d\varphi \{SS_I S_{II}; m_S m_I m_{II}\}$ , integrate over  $\theta$  and  $\varphi$ , sum over  $m_I$  and  $m_{II}$ , make use of the orthogonality and normalization of the spherical harmonics and the relation<sup>12</sup>

$$\sum_{m_I(m_{II})} \{SS_I S_{II}; m_S m_I m_{II}\} \\ \times \{S' S_I S_{II}; m_S m_I m_{II}\} = \delta_{SS'}, \quad (23)$$

and end up with a single one of the  $f_J(iLSr)$  on the left-hand side of the integro-differential equation. The right-hand member of this equation will, in general, contain radial functions  $f_J(jL'S'r)$  from all configurations and from values of  $L'$  and  $S'$  not necessarily the same as  $L$  and  $S$ . We can say at once from the invariance of the nuclear wave equation with respect to space rotations: firstly, that  $J$  and  $m_J$  have the same value on both sides of the equation; and secondly, that the equation for  $f_J(iLSr)$  must be independent of  $m_J$ —i.e., the right-hand side of the equation must contain as a factor the same expression  $\{JLS; m_J m m_S\}$  which appears on the left. (This could of course be proven with more difficulty directly from the expressions for  $\mathbf{V}_{ij}$ ,  $\mathbf{J}_{ij}$ ,  $\mathbf{I}_{ij}$ ). On introducing  $\rho$ ,  $\sigma$ ,  $\tau$  for polar coordinates of  $\xi$  (like the polar coordinates  $r$ ,  $\theta$ ,  $\varphi$  of  $\mathbf{X}$ ), and defining the  $J$ th components of  $\mathbf{V}$ ,  $\mathbf{J}$  (and similarly  $\mathbf{I}$ ) as follows:

$$\{JLS; m_J m m_S\} V_J(iLS; jL'S'; r) \\ = \int \sin \theta d\theta d\varphi \sum_{m_I(m_{II})} \sum_{m_I'(m_{II}')} Y_L^{(m)*}(\theta, \varphi) \\ \times \{SS_I^i S_{II}^i; m_S m_I m_{II}\} \mathbf{V}_{ij}(\mathbf{X}; m_I m_{II}; m_I' m_{II}') \\ \times \{JL'S'; m_J m' m_S'\} Y_{L'}^{(m')}(\theta, \varphi) \\ \times \{S' S_I^i S_{II}^i; m_S' m_I' m_{II}'\}; \\ \{JLS; m_J m m_S\} \mathbf{J}_J(iLSr; jL'S'\rho) \\ = r\rho \int \int \sin \theta d\theta d\varphi \sin \sigma d\sigma d\tau \sum \sum \dots \\ \times \mathbf{J}_{ij}(\mathbf{X} m_I m_{II}; \xi m_I' m_{II}') \dots, \quad (24)$$

we obtain the radial wave equations of the method of resonating group structure:

$$[(\hbar^2/2\mu_i)(d^2/dr^2 - L(L+1)/r^2) + E - E_i] f_J(iLSr) \\ = \sum_{jL'S'} \int H_J(iLSr; jL'S'\rho) f_J(jL'S'\rho) d\rho \\ = g_J(iLSr), \quad (25)$$

where  $g_J(iLSr)$  is an abbreviation for

$$\sum_{jL'S'} \{V_J(iLS; jL'S'; r) f_J(jL'S'r) \\ + \int [J_J - EI_J(iLSr; jL'S'\rho)] f_J(jL'S'\rho) d\rho\}. \quad (26)$$

## INTEGRAL EQUATIONS

### Reduction of integro-differential equations

In the radial integro-differential equations (25), we write

$$(2\mu_i/\hbar^2)(E - E_i) = -\kappa_i^2 \quad \text{for } E < E_i \\ \text{(configuration } i \text{ stable),} \\ (2\mu_i/\hbar^2)(E - E_i) = k_i^2 \quad \text{for } E > E_i \\ \text{(dissociation possible).} \quad (26)$$

We have the following cases to consider:

(A) All  $E_i > E$ . Completely stable nucleus. Sharp energy values.

(B) Only one  $E_i < E$ . Elastic collisions between groups  $I^i$  and  $II^i$ ; lifetime of compound nucleus determined by probability of a single mode of dissociation.

(C) More than one  $E_i < E$ . Elastic scattering; also transmutation processes  $I^i + II^i \rightleftharpoons I^j + II^j$ .

As illustration, Table I gives the configurations which may be used to describe the compound nucleus  ${}^4_2\text{He}$ :

<sup>12</sup> Wigner, reference 11, Eq. (28), p. 206.

TABLE I. Configurations of  ${}_2\text{He}^A$ .

$i$	$\mathbf{I}^i$	$S_{\mathbf{I}^i}$	$\mathbf{II}^i$	$S_{\mathbf{II}^i}$	$E_i$ (mMU)
1	$\text{H}^1$	$\frac{1}{2}$	$\text{H}^3$	$\frac{1}{2}$	-9.1
2	$n^1$	$\frac{1}{2}$	$\text{He}^3$	$\frac{1}{2}$	-8.1
3	$\text{H}^2$	1	$\text{H}^2$	1	-4.8

In case  $A$  (stable  ${}_2\text{He}^A$ ) the radial functions  $f$  must fall off exponentially for large  $r$  for all configurations; in addition, the  $f$ 's must satisfy the usual boundary condition  $f(0)=0$  at the origin. On considering the right hand members of (25) to be known functions<sup>13</sup> of  $r$ , we can immediately obtain expressions for the  $f_i$  satisfying the proper boundary conditions. We introduce the "regular" and "irregular" solutions of the homogeneous equation

$$[d^2/dr^2 - \kappa^2 - L(L+1)/r^2]f=0 \quad (27)$$

as follows:

$$\begin{aligned} \rho = \kappa r; \quad F_L(\rho) &= \rho^{L+1} \left( \frac{1}{\rho} \frac{d}{d\rho} \right)^L (\rho^{-1} \sinh \rho) \\ &= \{\rho^{L+1}/1 \cdot 3 \cdots (2L+1)\} \{1 + \rho^2/2(2L+3) + \cdots\}; \\ G_L(\rho) &= (-1)^L \rho^{L+1} \left( \frac{1}{\rho} \frac{d}{d\rho} \right)^L (\rho^{-1} \exp(-\rho)) \sim e^{-\rho}; \\ \frac{dF_L}{d\rho} G_L - F_L \frac{dG_L}{d\rho} &= 1; \end{aligned} \quad (28a)$$

and for later use write down also the regular and irregular solutions of the equation obtained by replacing  $-\kappa^2$  in (27) by  $k^2$ :

$$\begin{aligned} \rho = kr; \quad F_L(\rho) &= (-1)^L \rho^{L+1} \left( \frac{1}{\rho} \frac{d}{d\rho} \right)^L (\rho^{-1} \sin \rho) \\ &= \{\rho^{L+1}/1 \cdot 3 \cdots (2L+1)\} \cdot \{1 - \rho^2/2(2L+3) + \cdots\} \\ &\quad \sim \sin(\rho - L\pi/2); \\ G_L(\rho) &= (-1)^L \rho^{L+1} \left( \frac{1}{\rho} \frac{d}{d\rho} \right)^L (\rho^{-1} \cos \rho) \sim \\ &\quad \sim \cos(\rho - L\pi/2); \end{aligned}$$

$$\frac{dF_L}{d\rho} G_L - F_L \frac{dG_L}{d\rho} = 1. \quad (28b)$$

The uniquely determined solution of the inhomogeneous equation is

$$\begin{aligned} f_J(iLSr) &= -(2\mu_i/\hbar^2\kappa_i) \left\{ \int_0^r F_L(\kappa_i\sigma) G_L(\kappa_i r) \right. \\ &\quad \left. + \int_r^\infty F_L(\kappa_i r) G_L(\kappa_i\sigma) \right\} g(iLS\sigma) d\sigma. \end{aligned} \quad (29)$$

As the  $g$ 's are however given in terms of the  $f$ 's, we have cross relations which will not in general be consistent with each other—except for those special values of  $E$  which represent stable levels of the compound system. We write out (29) as a system of linear integral equations on the  $f$ 's:

$$\begin{aligned} f_J(iLSr) + \sum_{i'L'S'} \int_0^\infty S_J(iLSr; jL'S'\rho) \\ \times f_J(jL'S'\rho) d\rho = 0, \end{aligned} \quad (30)$$

where the kernel  $S_J$  is given by

$$\begin{aligned} S_J(iLSr; jL'S'\rho) &= (2\mu_i/\hbar^2\kappa_i) \\ &\times \left\{ \int_0^r G_L(\kappa_i r) F_L(\kappa_i\sigma) + \int_r^\infty F_L(\kappa_i r) G_L(\kappa_i\sigma) \right\} \\ &\times H_J(iLS\sigma; jL'S'\rho) d\sigma, \end{aligned} \quad (31)$$

and is therefore in principle known as soon as the  $\mathbf{V}$ 's,  $\mathbf{J}$ 's, and  $\mathbf{I}$ 's have been evaluated. We know from the theory<sup>14</sup> of integral equations that (30) has a characteristic solution only when the Fredholm determinant of the equation vanishes:

$$\begin{aligned} D(E) &= |\delta_{ij} \delta_{LL'} \delta_{SS'} \delta(r-\rho) \\ &\quad + S_J(iLSr; jL'S'\rho; E)| = 0. \end{aligned} \quad (32)$$

Eq. (32) determines the stable levels of the system. In diagonal expansion, it runs

$$\begin{aligned} D(E) &= 1 + \sum_{iLS} \int S(iLSr; iLSr) dr + (1/2!) \sum_{iLS} \sum_{i'L'S'} \iint \left| \begin{array}{cc} S(iLSr; iLSr) & S(iLSr; jL'S'\rho) \\ S(jL'S'\rho; iLSr) & S(jL'S'\rho; jL'S'\rho) \end{array} \right| dr d\rho \\ &\quad + \cdots = 0, \end{aligned} \quad (33)$$

<sup>13</sup> Cf. Mott and Massey, *The Theory of Atomic Collisions* (Oxford, 1933), p. 151, for an analogous method of conversion to an integral equation.

<sup>14</sup> Lovitt, *Linear Integral Equations* (New York, 1924), p. 41.



where for brevity the suffix  $J$  and the argument  $E$  have been omitted from  $S$ .

### ELASTIC SCATTERING

The collision of  $H^1$  and  $H^3$  with energy too small to form  $n^1+He^3$  comes under case  $B$ . For every given  $E$ , Eqs. (25) will now possess a solution. The wave functions for configurations 2 and 3 must still fall off exponentially for large  $r$ , but the  $f(1LSr)$ , which also satisfy the boundary condition at the origin, behave asymptotically for large  $r$  as combinations of  $\sin(k_1r)$  and  $\cos(k_1r)$ .<sup>15</sup>

A proton and triton without spin would be described at large distances by one function  $f_J(1J0r)$ . If this function is so normalized that that part of it which corresponds to the incoming wave  $e^{-i(k_1r-J\pi)}$  has amplitude  $-(1/2i)$ , then the amplitude of the outgoing wave  $e^{ik_1r}$  must have the same absolute value and may be written  $(1/2i)e^{2iK_J}$ . Here  $K_J$  is the so-called "phase shift," which is completely determined (up to  $\pm n\pi$ ) by the collision energy and form of the interaction, and which in turn, along with the other  $K_J$ 's, determines the differential cross section  $\sigma_{11}(\theta)$  for elastic scattering through the well known formula<sup>16</sup>

$$\sigma_{11}(\theta) = (4k_1^2)^{-1} \times \left| \sum_{L=0}^{\infty} (2L+1)(e^{2iK_L} - 1)P_L(\cos \theta) \right|^2. \quad (34)$$

### Effect of spin

The specific dynamic<sup>17</sup> action of nuclear spin splits up an incoming wave

$$-(1/2i) \exp[-i(k_1r - L\pi)],$$

containing two groups in one state  $JLS$  of specified spin orientation and given mutual angular momentum, into a number of outgoing waves representing these groups separating with altered spin orientations and changed mutual

<sup>15</sup> Provided we assume any coulomb fields to be broken off beyond some suitable distance  $r$ . The question of the most convenient procedure in this connection is discussed in more detail below.

<sup>16</sup> Mott and Massey, reference 13, p. 24.

<sup>17</sup> The statistical effect of the spin in a problem where two groups are identical (Mott, Proc. Roy. Soc. A126, 259 (1930)) is already taken into account in our treatment before the wave equation is reduced to radial form.

angular momentum. The particular solution  $f^{L,S}$  associated with the given initial conditions is a set of functions,  $g_J$  in number, having the asymptotic form:

$$\begin{aligned} f_J^{LS}(1LSr) &\sim -(1/2i) \exp[-i(k_1r - L\pi)] \\ &\quad + (1/2i)c_J(LS; LS) \exp[ik_1r], \\ f_J^{LS}(1L'S'r) &\sim (1/2i)c_J(L'S'; LS) \exp[ik_1r] \end{aligned} \quad (35)$$

$(L', S' \neq L, S).$

Another particular solution is obtained by letting the groups approach in a different initial state  $J\bar{L}\bar{S}$ ; altogether there are  $g_J$  such independent particular solutions for a given value of  $J$ . We therefore need  $g_J^2$  complex numbers  $c_J(L'S'; LS)$  to characterize completely the behavior at infinity of the independent solutions associated with a given component  $H_J$  of the interaction operator. For these large distances the waves associated with the stable configurations 2, 3,  $\dots$  have fallen to zero, and the total wave function for a state described by the quantum numbers  $J, m_J, L, S$  is obtained from

$$\begin{aligned} \chi_{Jm_J}^{LS}(\mathbf{1}, \mathbf{2}, \dots, \mathbf{N}) &= \sum_{L'S'} (1/kr) f_J^{LS}(1L'S'r) \\ &\quad \sum_{m_S'(m')} \{JL'S'; m_J m' m_S'\} Y_{L, (m')}(\theta, \varphi) \Phi^{1s', m_S'} \end{aligned} \quad (36)$$

by antisymmetrizing according to the procedure discussed earlier. However, in deriving the scattering cross section, as in the next paragraph, we are justified in dealing with the unsymmetrized  $\chi$ 's because: (1), the  $f_J$ 's are solutions of wave equations in which the  $H_J$ 's already include all dynamical effects of symmetrization (exchange interactions); and (2), those scattered waves in the total wave function which come from  $\chi$ 's differing by an interchange of particles between the constituent groups cannot interfere with each other at distances large in comparison with the size of the groups.

We consider a state typified by

$$\exp(i\mathbf{k}_1\mathbf{z})\Phi^{1s, m_S} + \text{scattered waves.} \quad (37)$$

The proper linear combination of the  $\chi_{Jm_J}^{LS}$  required to give this state is found most easily by comparing the coefficients of  $\exp[-i(k_1r$

$-L\pi]$  in the asymptotic expansions of the  $\chi$ 's and the advancing plane wave

$$\exp(ik_1 z) \sim \sum_L (2L+1) P_L(\cos \theta) (1/2ikr) \times [-e^{-i(k_1 r - L\pi)} + e^{ik_1 r}]. \quad (38)$$

For the comparison we use Eqs. (19) and (36). We find by application of the orthogonality relation<sup>18</sup>

$$\sum_J \{JLS; m_J m_S\} \{JLS; m_J m_S'\} = \delta_{mm'} \delta_{m_S m_S'} \quad (39)$$

and the equations of definition,

$$Y_L^{(m)}(\theta, \varphi) = \Theta_L^{(m)}(\theta) (2\pi)^{-\frac{1}{2}} e^{im\varphi}, \quad \Theta_L^{(0)}(\theta) = (L+1/2)^{\frac{1}{2}} P_L(\cos \theta), \quad (40)$$

that the desired coefficient of  $\chi_{Jm_J L S}$  is

$$\{JLS; m_S 0 m_S\} \delta_{m_S m_S'} [4\pi(2L+1)]^{\frac{1}{2}}. \quad (41)$$

The difference between the resultant linear superposition of solutions and the advancing plane wave is the scattered wave

$$(e^{ik_1 r}/2ik_1 r) \sum_L [4\pi(2L+1)]^{\frac{1}{2}} \times \left\{ \sum_{J L' S'} \sum_{m_S (m_S')} c_J(L' S'; LS) \{JLS; m_S 0 m_S\} \times \{JL' S'; m_S m' m_S'\} Y_{L'}^{(m')}(\theta, \varphi) \Phi^{1 S' m_S'} - Y_L^{(0)}(\theta, \varphi) \Phi^{1 S m_S} \right\}. \quad (42)$$

We square the absolute value of the coefficient of  $(e^{ik_1 r}/r) \Phi^{1 S' m_S'}$  and thus get the differential cross section for the process: groups in spin state  $\Phi^{1 S, m_S}$  collide and go off in the direction  $\theta, \varphi$  in the spin state  $\Phi^{1 S' m_S'}$ . The observable collision cross section, per unit solid angle, is obtained by averaging this over all  $(2S_I+1)(2S_{II}+1)$  initial modes of orientation and summing over all possible final values  $S' m_S'$ :

$$\sigma_{II}(\theta) = [(2S_I+1)(2S_{II}+1)4k_1^2]^{-1} \sum_{S, m_S} \sum_{S', m_S'} \left| \sum_L \left\{ \sum_{J L'} c_J(L' S'; LS) \{JLS; m_S 0 m_S\} \times \{JL' S'; m_S, m_S - m_S', m_S'\} (4L+2)^{\frac{1}{2}} \times \Theta_{L'}^{(m_S - m_S')}(\theta) - \delta_{S S'} \delta_{m_S m_S'} (2L+1) P_L(\cos \theta) \right\} \right|^2. \quad (43)$$

<sup>18</sup> Wigner, reference 11, Eq. (28).

### Determination of scattering matrix

Our next steps are based on the hope that all the desired quantities  $c_J(L' S'; LS)$  (for a fixed  $J$ ) can be obtained by consideration of a single generalized Fredholm determinant, without the necessity of actually constructing and investigating explicitly the asymptotic behavior of the solutions  $f_J^{LS}(1L' S' r)$ . We observe first of all that the transition from a set of integro-differential equations to a set of integral equations goes through as in the case of stable energy levels (Eq. (25) to Eq. (30)), since the two independent zero field solutions for positive energies (28b) have that same relation to their derivatives which made possible the building up of a Green's function in the earlier case. Only now the integral equations (30) are not unique, for the combination  $G_L(k_1 r) + [\text{ctg } K] F_L(k_1 r)$ , as well as  $G_L$  itself, satisfies (28b), and both are equally satisfactory in their asymptotic behavior for large  $r$ . Consequently, the kernel of (30) not only depends on the energy but in general also contains  $g_J$  undetermined "phase shifts"  $K_J(LS)$ :

$$S_J(iLSr; jL' S' \rho) = (2\mu_i/\hbar^2 k_i) \left\{ \int_0^r G_L(k_i \nu) F_L(k_i \sigma) + \int_r^\infty F_L(k_i \nu) G_L(k_i \sigma) + [\text{ctg } K_J(iLS)] \int_0^\infty F_L(k_i \nu) F_L(k_i \sigma) \right\} \times H_J(iLS\sigma; jL' S' \rho) d\sigma. \quad (44)$$

In this expression, the  $F$ 's and  $G$ 's represent the positive energy zero field solutions (28b) when  $E - E_i$  is positive (i.e., for configuration 1); but when  $E - E_i$  is negative (configurations 2, 3, ...), we understand  $k_i$  to be replaced by  $\kappa_i$  (Eq. (26)), and  $F$ 's and  $G$ 's to be the negative energy solutions (28a), and the  $\text{ctg } K_J(iLS)$  to be put equal to zero. We next remark that for *any* given energy the Fredholm determinant

$$D(E; K_J(1 \dots), \dots, K_J(1LS), \dots) = |\delta(iLSr; jL' S' \rho) + S(iLSr; jL' S' \rho)| \quad (45)$$

can be made to vanish, because we now have the  $K$ 's free to adjust, in contrast to the situation in the case of stable energy values. The equation  $D(E, K) = 0$  determines a  $g_J - 1$  dimensional

surface in the  $g_J$  dimensional space of the  $K$ 's. Every point on this surface corresponds to a particular solution for the radial wave functions  $f_J(iLSr)$ . This solution must be a linear combination with certain (complex) coefficients  $a_J^{LS}$  of the  $g_J$  particular solutions  $f_J^{LS}(iLSr)$  defined by Eq. (35). By comparison of the asymptotic behavior of the superposition of states,

$$\sum_{L, S} a_J^{LS} f_J^{LS}(iL'S'r) \sim -(1/2i)\delta_{ii} a_J^{L'S'} \times \exp[-i(k_1r - L\pi)] + (1/2i)\delta_{ii} \exp[ik_1r] \sum_{LS} c_J(L'S'; LS) a_J^{LS}, \quad (46)$$

with that of the solution of the integral equations (30) belonging to the kernel (44),

$$f_J(iL'S'r) \text{ asymptotically proportional to } \delta_{ii} \{ G_L(k_1r) + [\text{ctg } K_J(1L'S')] F_{L'}(k_1r) \} \text{ or to } \delta_{ii} \left\{ -(1/2i) \exp[-i(k_1r - L\pi)] + (1/2i) \exp[ik_1r] \frac{i \text{ctg } K - 1}{i \text{ctg } K + 1} \right\}, \quad (47)$$

we find

$$\sum_{L', S'} c_J(LS; L'S') a_J^{L'S'} = \exp[2iK_J(1LS)] a_J^{LS} \quad (48)$$

as the equations of connection between the coefficients  $a_J^{LS}$  and the points on the  $g_J - 1$  dimensional surface in the space of the  $K$ 's. It is seen that the constants  $c$  completely define the surface in question. The  $c$ 's form a unitary matrix, for the equality which must exist between the numbers of incoming and outgoing groups in the state (46) for arbitrary choice of the  $a$ 's,

$$k_1 \sum_{LS} |a_J^{LS}|^2 = k_1 \sum_{L'S'} \left| \sum_{LS} c_J(LS; L'S') a_J^{L'S'} \right|^2, \quad (49)$$

is just the necessary and sufficient condition<sup>19</sup> for unitary character.

Our problem is: To determine the unitary scattering matrix  $\|c_{mn}\|$  (we abbreviate by using  $m=1, 2, \dots, g$  to indicate the possible values of the pair  $L, S$ ), being given: (1), the surface

$$D(K_1, \dots, K_g) = 0 \quad (50)$$

<sup>19</sup> A. Wintner, *Spektraltheorie der Unendlicher Matrizen* (Leipzig, 1929), p. 34.

(from the Fredholm determinant of the integral equation); and (2), the equations

$$\sum_{\alpha=1}^g c_{m\alpha} a_\alpha = e^{2iK_m} a_m \quad (m=1, 2, \dots, g) \quad (51)$$

(which we have seen to be an equivalent way of representing the surface). We first eliminate the  $a$ 's by the condition that Eqs. (51) possess a solution:

$$\begin{vmatrix} c_{11} - e^{2iK_1} & c_{12} & \dots & c_{1g} \\ c_{21} & c_{22} - e^{2iK_2} & \dots & c_{2g} \\ \dots & \dots & \dots & \dots \\ c_{g1} & c_{g2} & \dots & c_{gg} - e^{2iK_g} \end{vmatrix} = 0. \quad (52)$$

Eq. (52) is a condition on the  $c$ 's which must be satisfied at every point  $K = (K_1, K_2, \dots, K_g)$  on the surface  $D(\mathbf{K}) = 0$ . In the actual applications the question of procedure depends upon whether the Fredholm determinant is available only by numerical calculations for each particular set of values of the  $K$ 's, or whether an analytic expression is obtainable for  $D$ . In the first case it is desirable for simplicity in the computations to restrict the  $K$ 's to real values, which, however, are not the most convenient in solving (52) for the  $c$ 's. In the second case, where we have an analytic expression for  $D$ , it is simplest to consider first those points on the surface which are defined by  $\text{ctg } K = i$  for all  $K$ 's except a particular  $K_m$ . The (complex) value of  $K_m = K_m'$  is then fixed by  $D(K) = 0$ , and from (52) we have at once  $c_{mm} = e^{2iK_m'}$ . In this way we find all diagonal elements of the unitary matrix. Next we let two  $K$ 's at a time vary freely, determining all other  $K$ 's by  $\text{ctg } K = i$ . Again we use (52) and find

$$c_{mn} c_{nm} = (c_{mm} - e^{2iK_m})(c_{nn} - e^{2iK_n}), \quad (53)$$

or in the limiting case  $\text{ctg } K_n \rightarrow i$ , where we can neglect  $c_{nn}$  in comparison with  $e^{2iK_n}$ ,

$$c_{mn} c_{nm} \rightarrow \left[ e^{2iK_m'} - e^{2i(K_m' + \delta K_m)} \right] \frac{1 - i(i + \delta \text{ctg } K_n)}{1 + i(i + \delta \text{ctg } K_n)};$$

that is,

$$c_{mn} c_{nm} = -4c_{mm} \frac{\partial K_m}{\partial(\text{ctg } K_n)} = 4c_{mm} \left[ \frac{\partial D_m}{\partial(\text{ctg } K_n)} / \frac{\partial D}{\partial K_m} \right]_{\text{ctg } K_n = i} \quad (m' \neq m). \quad (54)$$

If  $D(K_1, \dots, K_g)$  reduces to the product of two functions  $D'(K_1, \dots, K_a)$  and  $D''(K_{a+1}, \dots, K_g)$ , then the matrix  $\|c_{mn}\|$  breaks down to two square blocks along the diagonal, for from (54) and the unitary nature of  $c$  it follows that all elements  $c_{mn}$  connecting the one set of  $K$ 's with the other must be zero.

There is more than one<sup>20</sup> set of values for the  $c$ 's satisfying Eq. (52) for all points on the given surface: for example, the substitution  $u_{ik} = c_{ki}$  in general gives a new unitary matrix which is an equally good solution. Two matrices  $c$  and  $u$  both satisfy (52) only if the chain conditions

$$\begin{aligned} u_{ii} &= c_{ii}, \\ u_{ij}u_{ji} &= c_{ij}c_{ji}, \end{aligned} \tag{55a}$$

$$u_{ij}u_{jk}u_{ki} + u_{ik}u_{ki}u_{ji} = c_{ij}c_{jk}c_{ki} + c_{ik}c_{kj}c_{ji}, \text{ etc.},$$

are fulfilled for all values of the indices.

We suppose now that no off-diagonal elements vanish (trivial modifications ensue in the following if some are zero). We write the second chain condition, for  $i=1$ , in the form

$$\begin{aligned} u_{1j} &= \varphi_1^{-1}c_{1j}\varphi_j, \\ u_{j1} &= \varphi_j^{-1}c_{j1}\varphi_1 \quad [ = (\varphi_1c_{11}/c_{11})c_{1j}(\varphi_jc_{1j}/c_{j1})^{-1} ], \end{aligned} \tag{55b}$$

where the quantity  $\varphi_1$  is arbitrary and may be put equal to unity. Inserting (55b) in the third chain condition, with  $i=1$ , and using  $u_{jk}u_{kj} = c_{jk}c_{kj}$ , we find that there exist only two possible values for  $u_{jk}$ :

$$u_{jk} = \varphi_j^{-1}c_{jk}\varphi_k, \tag{55c}$$

$$u_{jk} = (\varphi_jc_{1j}/c_{j1})^{-1}c_{kj}(\varphi_kc_{1k}/c_{k1}). \tag{55d}$$

Similar solutions exist for  $u_{k1}$ , etc. Using the third chain condition in its general form, and recalling that the  $\varphi$ 's are arbitrary, we find that if  $u_{jk}$  is given by (55c), then all other  $u$ 's are given by the corresponding solution; and similarly for the second solution. In matrix language: If  $d$  is an arbitrary diagonal matrix with the general diagonal element  $d_{jj} = \varphi_j$  or  $d_{jj} = \varphi_jc_{1j}/c_{j1}$ , then the most general matrix  $u$  consistent with (52) is given by either

$$u = d^{-1}cd \quad \text{or} \quad u = d^{-1}c'd. \tag{55e}$$

We still have the information that  $u$ , as well as  $c$  and  $c'$ , is unitary, whence

$$\sum_j |c_{ij}|^2 \{ |\varphi_j|^2 - |\varphi_i|^2 \} = 0 \quad (i=1, 2, \dots, g).$$

With  $c_{ij} \neq 0$  for all  $i \neq j$  (cf. remark above), it follows by simple algebra that all  $|\varphi_j|^2$  must be equal; and since  $\varphi_1=1$ , we conclude that our diagonal matrix must be a phase matrix:  $d_{jj} = \varphi_j = e^{i\theta_j}$ . Therefore, given the Fredholm determinant (51), we can determine the scattering matrix  $\|c_{mn}\|$  uniquely up to a transformation by an arbitrary phase matrix and a possible interchange of rows and columns. In the trivial special cases mentioned above, where the off-diagonal elements of  $c$  vanish in such a way as to allow the scattering matrix to be broken up into submatrices, each block can have rows and columns interchanged independently of the other blocks.

When the conditions are satisfied for the time reversal of nuclear processes (absence of external magnetic fields, etc.), the matrix  $c$  shows a certain symmetry property equivalent to the principle of microscopic reversibility. The operation of time reversal,<sup>21</sup> in fact, converts a given wave function  $\Psi$  into a new one,  $K\Psi$ :

$$\begin{aligned} K\Psi(\mathbf{x}_1, \sigma_1, \dots, \mathbf{x}_m, \sigma_m, \mathbf{y}_1, \tau_1, \dots, \mathbf{y}_n, \tau_n) \\ = \mathbf{s}_{1x} \dots \mathbf{s}_{mx} \mathbf{t}_{1x} \dots \mathbf{t}_{nx} \Psi^*(\mathbf{x}_1, \sigma_1, \dots, \mathbf{y}_n, \tau_n) \\ = (-i)^{m+n} \sigma_1 \dots \sigma_m \tau_1 \dots \tau_n \Psi^*(\mathbf{x}_1, \sigma_1, \dots, \mathbf{y}_n, \tau_n), \end{aligned}$$

which, under the conditions stated, will be a linear combination of the old wave functions. We go back to (46), put  $a_J^{LS} = \bar{c}_J(L'S'; LS)$ , and obtain then solutions whose radial parts have the asymptotic behavior

$$\begin{aligned} f_J(iLSr) \sim \bar{c}_J(L'S'; LS)(1/2i) \\ \times \exp[-i(k_1r - L\pi)] \\ + (1/2i) \exp[ik_1r] \delta_{L'L} \delta_{S'S}. \end{aligned} \tag{56a}$$

The corresponding total wave function, after being operated on by the time reversal operator  $K$ , will also be a solution of the wave equation in the absence of external magnetic fields, etc., under which conditions we may suppose that the

<sup>20</sup> I am indebted to Professor H. Weyl and Professor J. H. M. Wedderburn for discussions of the arbitrariness in the  $c$ 's.

<sup>21</sup> Cf. E. Wigner, Göttingen Nachrichten **31**, 546 (1932), Eq. (10).

group functions satisfy

$$i^{2m} K \Phi_m = \Phi_{-m} \quad (56b)$$

(cf. Wigner's Eq. (21)). Then, using the relation<sup>21a</sup>

$$\{JLS; m_J m_L m_S\} = (-1)^{J-L-S} \\ \times \{JLS; -m_J, -m_L, -m_S\}, \quad (56c)$$

and referring to Eqs. (19) and (20), we have for the radial components of the new wave function

$$f_J^{(\text{new})}(iLSr) \sim (-1)^{J-S_1-S_{II}} (-i)^{2m_J} \\ \times \left\{ -(1/2i) \delta_{L'L} \delta_{S'S} \exp[-i(k_1 r - L\pi)] \right. \\ \left. + (1/2i) c_J(L'S'; LS) \exp[ik_1 r] \right\}. \quad (56d)$$

Comparison with the corresponding old radial wave function (35) gives

$$c_J(L'S'; LS) = c_J(LS; L'S'). \quad (57)$$

This relation shows that  $\|c_{mm}\|$  is a symmetric matrix, and with the help of (54) demonstrates that each element of the matrix is determined up to a factor  $\pm 1$ .

From the results of the last two paragraphs, we conclude that a knowledge of the Fredholm determinant (51) of our integral equations is sufficient, in the absence of external magnetic fields, to determine all elements of the scattering matrix up to a transformation by a diagonal matrix whose elements  $d_{ii}$  are  $\pm 1$ . Once this  $2^{g-1}$ -fold arbitrariness in choice of signs has been resolved for one energy, perhaps by explicit solution of the integral equations,<sup>22</sup> the principle of continuity with respect to variation of the energy is sufficient to determine the  $c$ 's completely for all energies from the Fredholm determinant,  $D(E; K_1, \dots, K_g)$  of the integral equation.

#### TRANSMUTATION

Cross sections giving the number and angular distribution of disintegration products may be calculated on the same line as the scattering probabilities considered above. The kernel of the integral equation is in fact given by the previous

expression (44), where now, however, several of the quantities  $E - E_i$  are positive, corresponding to the several possible unstable configurations or modes of disintegration of the compound nucleus. Associated with each unstable configuration  $i$  there are the phase shifts  $K_J(iLS)$ , related by the condition

$$D(E; K_J(1 \dots), \dots, K_J(iLS), \dots) = 0. \quad (58)$$

From the shape of the corresponding surface in  $K$  space and possibly by making explicit solutions of the integral equations in certain cases (see preceding discussion) we find the elements of a unitary matrix  $\|c_J(jL'S'; iLS)\|$  whose elements describe the asymptotic behavior of the particular solutions  $f_J^{iLS}(jL'S'r)$  of the wave equation:

$$f_J^{iLS}(jL'S'r) \sim -(1/2i) \delta_{i,j} \delta_{LL'} \delta_{SS'} \\ \times \exp[-i(k_j r - L\pi)] + (1/2i) (k_i/k_j)^{\frac{1}{2}} \\ \times c_i(jL'S'; iLS) \exp[ik_j r]. \quad (59)$$

The cross section per unit solid angle for the process in which groups  $I^i$  and  $II^i$  (for example,  ${}^2\text{He}^3$  and  ${}^0n^1$ ) collide with random spin orientation and groups  $I^j$  and  $II^j$  ( ${}^1\text{H}^3$  and  ${}^1\text{H}^1$ ) separate along a line oriented at an angle  $\theta$  with respect to the original direction is

$$\sigma_{ij}(\theta) = [(2S_{I^i} + 1)(2S_{II^i} + 1)4k_i k_j]^{-1} \sum_{S, m_S} \sum_{S', m_{S'}} \\ \times \left| \sum_{J, L, L'} c_J(jL'S'; iLS) \{JLS; m_S 0 m_S\} \right. \\ \left. \times \{JL'S'; m_S m_S - m_{S'} m_{S'}\} (4L + 2)^{\frac{1}{2}} \right. \\ \left. \times \Theta_{L', (m_S - m_{S'})}(\theta) \right|^2 \quad (i \neq j), \\ \sigma_{ii}(\theta) = \sigma_{ii} \quad (\text{Eq. (43)}). \quad (60)$$

#### DISCUSSION

##### Validity of treatment

The connection which we have obtained between the scattering and disintegration cross sections and a certain surface

$$D(E; K_1, \dots, K_g) = 0$$

defined by the Fredholm determinant of an integral equation, does not depend for its

<sup>21a</sup> This relation was suggested by Professor Wigner, who has also been kind enough to clear up several points in connection with Eqs. (55e) and (57).

<sup>22</sup> Cf. remarks in discussion.

validity on the accuracy of what we have called the method of resonating group structure. The derivation, in fact, made use only of certain quite general asymptotic properties of the solution of the wave equation. Consequently, the same method of treatment goes through also in the case where that kernel is employed in the integral equation (30) which will give the rigorous solution of the problem in question—i.e., a kernel  $S$ , built up somewhat as (44), but from the accurate wave functions of the individual groups and the accurate solutions of the problem of  $N$  free neutrons and protons, followed by the energy operator  $H$  representing individual particle rather than group interactions. It appears feasible to carry out such a treatment of the nuclear three-body problem in detail.

**Numerical calculations**

However the fundamental integral equation is derived, the central problem from the computational point of view is to evaluate the associated Fredholm determinant. A diagonal expansion on analytic lines, following Eq. (33), is not in general possible, although the possibility is not excluded of finding a suitable analytic approximation to  $S$ , such that the powers,  $S^n$ , can be evaluated explicitly.

A straightforward numerical calculation offers another procedure, which can always be carried through to a finish. For a simple illustration, we suppose that the system in question is to be described by a single configuration, in which the two groups have no spin. The range of values of the intergroup separation,  $r=0$  to  $r=r^*$ , over which the interaction departs appreciably from its asymptotic value, is replaced by the set of points  $r_1=a, r_2=2a, \dots, r_p=pa$ , the spacing,  $a$ , being taken sufficiently small. The integral equation

$$f(r) + \int S(r, \rho)f(\rho)d\rho = 0 \tag{30'}$$

may then, by Simpson's rule, be replaced approximately by the set of linear equations

$$f_i + \sum_{\alpha=1}^p S_{i\alpha}f_\alpha = 0, \quad (i=1, 2, \dots, p), \tag{30''}$$

where

$$f_1=f(a), \quad f_2=f(2a), \quad \dots$$

and

$$\begin{aligned} S_{11} &= (2a/3)S(a, a), \quad S_{12} = (4a/3)S(a, 2a), \\ S_{13} &= (2a/3)S(a, 3a), \quad \dots \tag{30'''} \\ S_{21} &= (2a/3)S(2a, a), \quad \dots, \quad \text{etc.} \end{aligned}$$

The kernel  $S$  may itself be calculated by a similar procedure of approximation to Eq. (44):

$$S_{mn} = \sum_{\alpha=1}^p G_{m\alpha}H_{\alpha n}. \tag{44''}$$

Here the matrix  $\|G_{mn}\|$  bears the same type of relation to the function

$$\begin{aligned} G(r, \rho) &= (2\mu/\hbar^2k) \{ G_L(kr)F_L(k\rho) \\ &\quad + \text{ctg } KF_L(kr)F_L(k\rho) \} \quad (\rho < r) \\ &= (2\mu/\hbar^2k) \{ G_L(k\rho)F_L(kr) \\ &\quad + \text{ctg } KF_L(kr)F_L(k\rho) \} \quad (\rho > r) \end{aligned} \tag{44'''}$$

that  $\|S_{mn}\|$  bears to  $S(r, \rho)$ , except for one detail. Since  $G(r, \rho)$  has a kink (discontinuous first derivative) at the point  $\rho=r$ , the Simpson coefficients  $2/3, 4/3$ , etc., must be slightly modified to make the summation (44'') give the best agreement with the integration of (44). Written following the order of (30'''), the proper coefficients for the calculation of the matrix  $G$  are

$$\begin{aligned} &2a/3, \quad 4a/3, \quad 2a/3, \quad 4a/3, \quad 2a/3, \quad 4a/3, \quad 2a/3, \quad \dots \\ &9a/8, \quad 6a/8, \quad 9a/8, \quad 9a/8, \quad 17a/24, \quad 4a/3, \quad 2a/3, \quad \dots \\ &2a/3, \quad 4a/3, \quad 2a/3, \quad 4a/3, \quad 2a/3, \quad 4a/3, \quad 2a/3, \quad \dots \\ &17a/24, \quad 9a/8, \quad 9a/8, \quad 6a/8, \quad 9a/8, \quad 9a/8, \quad 17a/8, \quad \text{etc.} \end{aligned}$$

In order for (30'') to possess a solution, the Fredholm determinant

$$D(E, K) = \begin{vmatrix} 1 + S_{11} & S_{12} & \dots & \dots \\ S_{21} & 1 + S_{22} & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & 1 + S_{pp} \end{vmatrix}$$

must vanish. For stable states ( $E < 0$ ,  $\text{ctg } K = 0$ ) the Fredholm determinant is evaluated for one energy value, then another, and so on; the curve  $D(E)$  as a function of energy crosses the horizontal axis at the eigenwerte. The case of scattering (and in general, disintegration) is treated in the same way.

Though laborious, it is quite feasible to deal with determinants of the 30th order. The proce-

dure of evaluation is straightforward on a calculating machine:<sup>23</sup> The lowest row ( $d_{p1}, d_{p2}, \dots, d_{pp}$ ) (we abbreviate  $\delta_{ik} + S_{ik}$  by  $d_{ik}$ ) is multiplied by  $(d_{p-1, p}/d_{pp})$  and subtracted from the  $(p-1)$ th; by  $(d_{p-2, p}/d_{pp})$  and subtracted from the  $(p-2)$ nd row, etc. When all elements in the  $p$ th column are reduced to zero, (except  $d_{pp}$ ), the (new) second row is used in the same way to eliminate all elements in the  $(p-1)$  the column except  $d_{p, p-1}$  and  $d_{p-1, p-1}$ ; and so on. The value of the determinant is given by the product of the diagonal elements of the final matrix:  $D = d_{11}'d_{22}' \dots d_{pp}'$ . If this vanishes, the wave function (vector)  $f$  may easily be found, if desired, by recursive solution:  $f_1 = 1$ ;  $f_2 = -d_{21}'f_1/d_{22}'$ ;  $f_3 = -(d_{31}'f_1 + d_{32}'f_2)/d_{33}'$ , etc. The smoothness of the curve  $f(r)$  drawn through the values so obtained furnishes a good check on the calculations.

#### Modifications in procedure

So far we have assumed that the interaction falls off rapidly. If it follows the Coulomb law for large distances, then in the calculations we may take it to be broken off at  $r = r^*$ . The asymptotic form of the wave functions we obtain in this way corresponds to zero field from  $r^*$  to  $\infty$ ; we then fit the Coulomb functions on at  $r^*$ , in such a way<sup>24</sup> as to have the same logarithmic derivative as those combinations of zero field solutions described by the phase shifts  $K$ . This procedure determines the phase shifts  $K'$  of the solution for the actual field, measured with respect to the solutions for a pure Coulomb field. The scattering cross section is known<sup>25</sup> in terms of  $K'$ , for the case of elastic collisions with zero spin, and may be derived for scattering and disintegration processes involving groups with spin along the lines described above. An alternative procedure, using for  $F_L$  and  $G_L$  the Coulomb wave functions, would require more detailed tables of these functions than are now available.

In the actual problems treated so far by the method we have described, it appears to be a general rule that the larger the number of par-

ticles involved, the more closely

$$\int \sum_{iL'S'} I_J(iL'Sr; jL'S'\rho) f_J(jL'S'\rho) d\rho$$

approaches to being the negative of  $f_J(iL'Sr)$ , although of course the operator  $\delta_{ij}\delta_{LL'}\delta_{SS'}\delta(r-\rho) + I_J(\dots)$  is always positive definite. This behavior is connected with the large number of nodes present in the total wave function  $\Psi$  owing to its antisymmetry properties. In fact,  $\int \Psi^* \Psi d\tau$  is very much smaller than the integral  $\int \chi^* \chi d\tau$  of any one of the (not antisymmetrized) parts  $\chi$  (Eq. (36)) from which  $\Psi$  is built up, and this comes to expression in the feature we have mentioned. The appearance of the operator  $\delta + I$  in the denominator of the expectation value of the energy has the consequence that calculations are sensitive to the accuracy with which  $\int \int f^*(r) [\delta(r-\rho) + I(r, \rho)] f(\rho) dr d\rho$  is determined. This would suggest that  $\varphi = [\delta + I]^{-1/2} f$  be introduced as dependent variable, instead of  $f$  itself; for  $\varphi$  has the same asymptotic behavior as  $f$  and gives  $\int \varphi^*(r) \varphi(r) dr$  for the integral in question. The method is known by which the positive square root of a positive definite Hermitian matrix may be obtained,<sup>26</sup> but we do not carry out here the consequences of this possible improvement on the procedure we have already described.

The development above was given in detail only for configurations consisting of two groupings. When three groupings interact, one approximate mode of description is to regard the configuration as composed of two groupings, the internal wave function of one of which is in turn determined by the method of resonating group structure. More accurate, also more symmetric, is the direct extension to three bodies of the type of kernel we have used for two. Instead of the functions  $F_L, G_L$  of one variable,  $r$ , we must then have a combination of functions of three variables  $r_{12}, r_{13}, r_{23}$  built up into a Green's function for the "radial" motion of three free bodies, the angular part of the motion having been separated out by known<sup>27</sup> methods.

<sup>23</sup> Cf. James and Coolidge, J. Chem. Phys. **1**, 834 (1933).

<sup>24</sup> See John A. Wheeler, "Wave Functions for Large Arguments by the Amplitude Phase Method," Phys. Rev. **52**, 1123 (1937).

<sup>25</sup> Cf. Mott and Massey, reference 13, p. 275.

<sup>26</sup> Cf. M. Born and P. Jordan, *Elementare Quantenmechanik* (Berlin, 1930), p. 69.

<sup>27</sup> Cf. G. Breit, Phys. Rev. **35**, 569 (1930), and especially J. O. Hirschfelder and E. Wigner, Proc. Nat. Acad. **21**, 113 (1935), where the corresponding separation of angles is treated in the case of  $N$  bodies.

By introducing a dependence of the individual group wave functions on the intergroup distances, we get an approximation to the total wave function which corresponds to better values for the absolute energy than is otherwise obtained. In some ways this modification is analogous to a polarization effect, but it must be remembered that the interaction between the various groups is far too intimate for such a simple change to make the total wave function really approach in full detail to the accurate solution of the given quantum mechanical problem. Rather such a refinement is to be taken in the spirit of the method of resonating group structure, in which we try to build up a suitable description of the whole system from what we know of its parts, being guided throughout by the variation principle. Use of a "polarized" group wave function appears to be especially suitable in treating such a problem as that of proton-deuteron collisions. On the other hand there are situations (as when the available energy is large) where it is more convenient, and indeed absolutely necessary, to take into account excited group states in making the proper allowance for the interaction between the various groups (we use the word "group" here in the extended sense employed throughout the present discussion, in which there is no one to one correspondence between a given group and definite neutrons and protons picked out of the total system). Analogy with the polarization problem in atomic physics make it clear that explicit dependence of wave functions on separation, and excitation of higher states are to a considerable extent even in the nuclear problem equivalent ways of allowing for the same thing, and indeed the mathematical treatment given

above indicated that it was practically impossible to introduce both methods of description at the same time in a consistent manner. The question as to which excited states of the individual groups are most important in the description of the compound system is of course an important one in the actual applications, and has received so far only a very general kind of answer.<sup>28</sup>

A thoroughgoing treatment of collision processes for nuclei of medium and high atomic weight in the detail we have mentioned in this paper appears to be out of the question. The considerations of Bohr<sup>29</sup> point rather to a statistical approach, based on the analogy between nuclear structure and the liquid state, as more fruitful. For this reason a study of the detailed correspondence between the two viewpoints would be very valuable. In this connection the importance of symmetry arguments has already been pointed out.<sup>28</sup>

For sufficiently light nuclei, on the other hand, the connection between nuclear forces and observations on collisions and transmutations can be traced out with sufficient accuracy to make possible definite conclusions about the interactions involved. The method of resonating group structure described above has been used to treat the interaction between two normal alpha-particles,<sup>30</sup> and is being applied to other problems,<sup>31</sup> where further details will be given.

<sup>28</sup> Preceding paper.

<sup>29</sup> Niels Bohr, *Nature* **137**, 344 (1936); also unpublished lectures summarized in *Science* **86**, 161 (1937).

<sup>30</sup> To be published.

<sup>31</sup> Four-particle problem: preliminary report, Hermon Parker, Paper No. 3, Chapel Hill-Durham meeting of the American Physical Society, Feb. 19-20, 1937. Five-particle problem: Miss K. Way, University of North Carolina, in progress.