trated in Fig. 1. In the calculation given in Table II, v was taken as 0.22, 0.7, 0.6 for Fe, Co, and Ni, respectively, these values being required by the observed values of the saturation magnetization.

The calculated ratio β^2/γ is compared with the empirical W' in the last two rows of Table II. In spite of the approximate nature of the estimates leading to the values for β^2/γ, these values are satisfying in two respects. As we pass from Fe through Co to Ni, β^2/γ increases in approximately the same manner as does W'. For each metal the calculated β^2/γ is somewhat larger than the empirical W', thereby allowing for a negative contribution from the coefficient α. We conclude that the model for ferromagnetism proposed in the first paper of this series gives a satisfactory quantitative interpretation of the Weiss constant.

A Variational Approach to Nuclear Reactions

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The formalism of Wigner and Eisenbud for nuclear reactions is carried out by means of a variation principle. A variation principle of the Hulthén type is derived for the R matrix and applied to trial wave functions written in terms of the resonance functions, X_λ, of the Wigner-Eisenbud formalism. As a result, a finite level formula for the R matrix is directly obtained.

I. INTRODUCTION AND SUMMARY

IN a paper by Wigner and Eisenbud,[1] general equations describing nuclear reactions are rigorously derived. The essential result of the theory is the expression which the authors obtain for a matrix which they call the R matrix. The R matrix is a real, symmetric matrix whose rows and columns are labeled according to the possible alternatives of the reaction. From the R matrix one may directly calculate the collision matrix, which gives the cross sections of the possible reactions according to $\sigma_{ss'} = \pi k_s^{-2} |\delta_{ss'} - U_{ss'}|^2$, where $\sigma_{ss'}$ is the cross section of the reaction going from the sth pair of particles to the s'th pair and $U_{ss'}$ is the corresponding element of the collision matrix. The R matrix is related to the collision matrix of the reaction by an equation of the form $U = \omega(1 + ijRj)(1 - ijRj)^{-1}\omega$, where j and ω are, respectively, real diagonal and unitary diagonal matrices. The elements of the j and ω-matrices depend only on non-nuclear parameters, in that they involve only constants which enter into the solutions of the two-body Schrödinger equation in the regions of configuration space where there are two distinct reaction products. The calculation of the collision matrix from the R matrix may therefore be accomplished in a straightforward manner without any additional information about the compound nucleus other than that which is contained in the R matrix. This paper will concern itself only with the R matrix.

An expression for the R matrix will be obtained on the basis of a variational calculation. The variation principle is of the same general type as that derived by Hulthén[2] for the two-body quantum-mechanical scattering problem. The derivation presented here is along lines similar to those followed by W. Kohn[3] in a recent paper.

The variation principle is applied to a trial wave function, which is written in terms of a finite number of functions, X_λ, defined in W-E. These functions are intended to represent the resonance states of the compound nucleus. Upon making the variational expression stationary with respect to variations of the coefficients of the X_λ, one obtains directly an expression for the R matrix in terms of the states used in the trial wave function. The variationally derived expression for the R matrix is in agreement with the rigorous expression for the R matrix up to the order of the number of terms used in the trial wave function. Moreover, the variationally derived R matrix is real and symmetric for all trial wave functions of the type considered.

The notation used in this paper will be essentially the same as the notation of W-E. This has two advantages. First, it gives the present work all of the generality of W-E in that arbitrary long-range interactions and arbitrary angular momenta are allowed. Second, it allows for a direct comparison between the results of the variational calculation and the rigorous result.

In order to carry out this work it will be necessary to present a brief description of the Wigner-Eisenbud formalism. This will be done in Sec. II. Section III is

[1] E. P. Wigner and L. Eisenbud, Phys. Rev. 72, 29 (1947). This reference will be referred to as W-E throughout the remainder of this work.
[2] L. Hulthén, Extrait, Dixième Congrès des Mathematiciens Scandinaves, Copenhague, 1946.
[3] W. Kohn, Phys. Rev. 74, 1763 (1949).

devoted to the derivation of the variation principle for the R matrix. In Sec. IV, the variation principle is applied to a trial wave function and an expression for the R matrix is derived.

II. THE WIGNER-EISENBUD FORMALISM

Wigner and Eisenbud divide the configuration space of all particles of the reacting system into an external region and an internal region. The external region is defined as the region of space where the wave function may be written as the product of the internal wave function of two nuclear reaction products with a function of the distance between their centers of mass, r_s, and the corresponding direction, Ω_s. The remainder of configuration space is called the internal region. It is in the internal region that one speaks of the compound nucleus as being formed, as there all particles are close together.

A distinct way in which the compound nucleus may decay is called an alternative of the reaction. An alternative, denoted by the index s, is specified by the composition of the resulting nuclei (the number of neutrons and protons in each), their state of excitation, their relative orbital angular momentum, and their composite spin (all of this for a fixed total angular momentum and z component of the total angular momentum). For definiteness, let us say that the hypersurface, S, which separates the internal from the external region is defined by $r_s = a_s$ (all s), where the a_s are chosen large enough so that the above statements about the external region are true.

Two independent solutions, in the part of the external region corresponding to the sth alternative, are written

$$D_s = (S_s(r_s)/r_s)\psi_s(i_s, \Omega_s), \quad V_s = (C_s(r_s)/r_s)\psi_s(i_s, \Omega_s), \quad (1)$$

where i_s stands for the internal coordinates of the two nuclei of the sth alternative. The function $\psi_s(i_s, \Omega_s)$ is the product of the internal wave function of the nuclei of the sth alternative with the angular part of their relative motion. It is normalized according to

$$\int |\psi_s(i_s, \Omega_s)|^2 di_s d\Omega_s = 1. \quad (2)$$

Furthermore, these functions may be shown to be orthogonal to each other on S, i.e.,

$$\int \psi_{s'}^*(i_{s'}, \Omega_{s'})\psi_s(i_s, \Omega_s)dS = a_s^2 \delta_{ss'}. \quad (3)$$

$S_s(r_s)/r_s$ and $C_s(r_s)/r_s$ are two independent solutions of the radial part of the Schrödinger equation for the sth alternative. They are specified by the boundary conditions,[4]

$$\begin{aligned} S_s(a_s) &= 0, & C_s(a_s) &= (M_s/\hbar)^{\frac{1}{2}}, \\ dS_s(a_s)/dr_s &= (M_s/\hbar)^{\frac{1}{2}}, & dC_s(a_s)/dr_s &= 0. \end{aligned} \quad (4)$$

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[4] These boundary conditions are simpler than the original boundary conditions used in W-E, which Wigner later found to be unnecessarily complicated.

Here M_s is the reduced mass of the two reaction products specified by the index s.

If there are n alternatives, then it is clear that there are n linearly independent solutions (corresponding to the n-fold arbitrariness in the choice of the incident currents for the alternatives) of the wave equation for a given set of the constants of the motion. A set of independent solutions may be chosen which in the external region are written

$$\phi_s = D_s + \sum_{s'=1}^{n} R_{ss'} V_{s'}. \quad (5)$$

The $R_{ss'}$ are the elements of the R matrix. It is shown in W-E that they may be taken to be real without loss of generality.

The solutions ϕ_s are expanded in the internal region in terms of a complete set of eigenfunctions, X_λ, of the hamiltonian of the entire system, which satisfy the hermitian boundary condition at S:

$$-(1/a_s)\int \psi_s(i_s, \Omega_s)X_\lambda^* dS$$
$$= \int \psi_s(i_s, \Omega_s) \operatorname{grad}_n X_\lambda^* dS. \quad (6)$$

The X_λ are normalized to unity within the internal region. The corresponding eigenvalue is called E_λ. It should be noted that the boundary condition satisfied by X_λ at the part of S corresponding to $r_s = a_s$ is essentially the same as the boundary condition fulfilled by V_s.

In the internal region one then writes

$$\phi_s = \sum_{\lambda=1}^{\infty} a_{s\lambda} X_\lambda; \quad a_{s\lambda} = \int_{\substack{\text{internal} \\ \text{region}}} X_\lambda^* \phi_s d\tau. \quad (7)$$

If one applies Green's theorem to ϕ_s and X_λ over the internal region, one obtains

$$a_{s\lambda} = (\tfrac{1}{2}\hbar)^{\frac{1}{2}}\gamma_{\lambda s}/(E_\lambda - E), \quad (8)$$

where

$$\gamma_{\lambda s} = (2/\hbar)^{\frac{1}{2}}(\hbar^2/2M_s)\int X_\lambda^* V_s dS. \quad (9)$$

The $\gamma_{\lambda s}$, too, may be taken to be real without loss of generality. Upon equating the expansion of ϕ_s within the internal region to the value of ϕ_s on S given by Eq. (5), one obtains, with the aid of Eqs. (3) and (9)

$$R_{ss'} = \sum_{\lambda=1}^{\infty} \frac{\gamma_{\lambda s}\gamma_{\lambda s'}}{E_\lambda - E}. \quad (10)$$

This is the fundamental result of the theory. The dependence of the elements of the R matrix upon the energy is exhibited, as the $\gamma_{\lambda s}$ and the E_λ are energy-independent quantities.

It should be mentioned that if one approximates the $R_{ss'}$ by one of the terms in the infinite series, the cross

section (calculated from the relationship stated in Sec. I) takes the form of the usual one-level resonance formula.

III. VARIATION PRINCIPLE FOR THE R MATRIX

A variation principle for the R matrix of a nuclear reaction is derived in this section. The variation principle is applicable to the same class of reactions to which the Wigner-Eisenbud formalism applies.

We shall consider variations of the expression

$$I_{ss'} = \int \phi_{s'}{}^* (H-E) \phi_s d\tau \qquad (11)$$

for independent variations of the ϕ_s and $\phi_{s'}{}^*$ about the corresponding solutions, given in the external region by Eq. (5). Here, H is the hamiltonian of the entire nuclear system and E is the total energy. The integration with respect to τ indicates integration over the coordinates of all particles of the system (including spin coordinates). The variations of the wave functions which will be considered will be of a restricted type. Only varied wave functions which, in the external region, have the same form as the corresponding true solutions, Eq. (5) will be considered. That is, only arbitrary variations of the elements of the R matrix are allowed in the external region. The variations of the wave function in the external region are therefore written

$$\delta\phi_s = \sum_{s''} (\delta R_{ss''}) V_{s''}, \quad \delta\phi_{s'}{}^* = \sum_{s''} (\delta R_{s's''}{}^*) V_{s''}{}^*. \quad (12)$$

On the other hand, in the internal region, one allows arbitrary variations of the wave function.

The variation of $I_{ss'}$ resulting from independent variations of ϕ_s and $\phi_{s'}{}^*$ is then

$$\delta I_{ss'} = \int \delta\phi_{s'}{}^* (H-E)\phi_s d\tau + \int \phi_{s'}{}^* (H-E)\delta\phi_s d\tau. \quad (13)$$

As $(H-E)D_s = (H-E)V_s = 0$, the above integrals, in view of the restricted nature of the allowed trial wave functions in the external region, may be taken over the internal region alone. In order to obtain a stationary expression, the order of $\phi_{s'}{}^*$ and $\delta\phi_s$ must be reversed in the second integral of the above equation. This may be done by applying Green's theorem over the internal region. There will be contributions from the surface integral over S which may be evaluated from the boundary values of the functions D_s and V_s. The contribution to the surface integral from the part of S corresponding to the s'' alternative is

$$-\frac{\hbar^2}{2M_s}\int \left\{ (D_{s'}{}^*\delta_{s's''} + R_{s's''}{}^* V_{s''}{}^*)\frac{\partial}{\partial r_{s''}} \right.$$

$$\times (\delta R_{ss''} V_{s''}) \Big|_{r_{s''}=a_{s''}} - (\delta R_{ss''} V_{s''})\frac{\partial}{\partial r_{s''}}$$

$$\left. \times (D_s{}^*\delta_{s's''} + R_{s's''}{}^* V_{s''}{}^*) \Big|_{r_{s''}=a_{s''}} \right\} dS.$$

Here we have made use of the fact that D_s and V_s, or $\psi_s(i_s, \Omega_s)$, are appreciable only on the part of S for which $r_s = a_s$. For this reason, too, the integral in the above expression may be taken over the entire surface.[5] Using Eqs. (1), (3), and (4) and summing over s'', one obtains for the surface integral

$$\tfrac{1}{2}\hbar\delta R_{ss'}.$$

Equation (13) may then be written

$$\delta(I_{ss'} - \tfrac{1}{2}\hbar R_{ss'}) = \int \delta\phi_{s'}{}^* (H-E)\phi_s d\tau$$

$$+ \int \delta\phi_s [(H-E)\phi_{s'}]{}^* d\tau. \quad (14)$$

As the right side of the above is zero, the variation principle is

$$\delta(I_{ss'} - \tfrac{1}{2} R_{ss'}) = 0. \quad (15)$$

As $I_{ss'}$ is zero for the true solutions, the above is a stationary expression for the elements of the R matrix and may be used for variational calculations of any of the elements. It should be recalled, however, that in applying the variation principle, the trial wave functions used must have the form stated in Eq. (5) in the external region.

IV. VARIATIONAL CALCULATION OF THE R MATRIX

In this section the R matrix is calculated on the basis of the variation principle stated in Eq. (15). In the internal region the trial wave functions are written in terms of a finite number of the resonance functions X_λ. We write the trial functions

$$\phi_s{}^{(\xi)} = \sum_{\lambda=1}^{\xi} a_{\lambda s} X_\lambda \qquad \text{(internal region)}, \quad (16a)$$

$$\phi_s{}^{(\xi)} = D_s + \sum_{s'} R_{ss'}{}^{(\xi)} V_{s'} \qquad \text{(external region)}. \quad (16b)$$

The $a_{\lambda s}$ are unknown parameters to be determined from the variation principle and ξ, the number of resonance functions used in the trial wave functions, will be called the order of the trial wave function. In Eq. (16b), the $R_{ss'}{}^{(\xi)}$ are the trial values for the elements of the R matrix. They are expressed in terms of the coefficients, $a_{\lambda s}$, by equating the expression for the trial wave function in the external region to the expression for the trial wave function in the internal region at the

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[5] This, of course, is also the explanation of the orthogonality relation on S, Eq. (3), which for indices corresponding to alternatives of different compositions is actually only approximately true. It becomes rigorously true only if one allows the surface S to become indefinitely large. In spite of this, the variation principle will be rigorously, not approximately, true. This may be seen by applying Green's theorem to a larger surface geometrically similar to S. The orthogonality relations then become rigorously true and the evaluation of the surface integral yields the same result.

surface, S. One obtains

$$\sum_{\lambda=1}^{\xi} a_{\lambda s}X_\lambda = \sum_{s'} R_{ss'}^{(t)} V_{s'} \quad \text{(on } S),\qquad(17)$$

where use has been made of the fact that D_s is zero on S. Multiplying Eq. (17) by V_s^* and integrating over S, one obtains with the aid of Eqs. (1), (3), (4), and (9)

$$R_{ss'}^{(t)} = \left(\frac{2}{h}\right)^{\frac{1}{2}} \sum_{\lambda=1}^{\xi} a_{\lambda s}\gamma_{\lambda s'}.\qquad(18)$$

At this point a word should be said about an apparent peculiarity of this trial wave function. As it is written, the trial wave functions has a discontinuity in its first derivative at S. As the V_s match the X_λ at S, and as they both satisfy the same boundary condition there, it is clear that they will match in their first derivatives as well. Therefore, the first derivative of D_s at S will not be matched. The discontinuity is of course a consequence of the fact that all of the X_λ satisfy the same hermitian boundary condition at S. Therefore, if one wishes to use only the X_λ in the internal region, the discontinuity is unavoidable in view of the fact that the trial wave functions must have the form that they do in the external region. The operation of the second derivative in the hamiltonian on such a trial wave function will give a finite contribution to the integral in the stationary expression in an infinitesimal volume element about the surface S. Such a contribution is evaluated according to

$$\lim_{\epsilon\to 0}\int_{a-\epsilon}^{a+\epsilon} \frac{d^2 f}{dr^2}dr = \lim_{\epsilon\to 0}\frac{df}{dr}\Big|_{r=a-\epsilon}^{r=a+\epsilon}.$$

This additional contribution to the integral, $I_{ss'}$, is therefore,

$$\text{surface term of } I_{ss'} = -\frac{\hbar^2}{2M_s}\int \phi_{s'}^{(t)*}\frac{\partial}{\partial r_s}D_s dS$$

$$= -\frac{\hbar^2}{2M_s}\int \phi_{s'}^{(t)*} V_s dS$$

$$= -\left(\frac{\hbar}{2}\right)^{\frac{1}{2}} \sum_{\lambda=1}^{\xi} a_{\lambda s'}^* \gamma_{\lambda s}.\qquad(19)$$

The contribution to $I_{ss'}$ from the interior is

$$\text{volume term of } I_{ss'} = \sum_{\lambda=1}^{\xi} a_{\lambda s'}^* a_{\lambda s}(E_\lambda - E).\qquad(20)$$

Using Eqs. (18), (19), and (20), the stationary expression, written as a function of the $a_{\lambda s}$ and $a_{\lambda s'}^*$ is

$$I_{ss'} - \frac{\hbar}{2}R_{ss'} = \sum_{\lambda=1}^{\xi} a_{\lambda s'}^* a_{\lambda s}(E_\lambda - E) - \left(\frac{\hbar}{2}\right)^{\frac{1}{2}} \sum_{\lambda=1}^{\xi} a_{\lambda s'}^* \gamma_{\lambda s}$$

$$-\left(\frac{\hbar}{2}\right)^{\frac{1}{2}} \sum_{\lambda=1}^{\xi} a_{\lambda s}\gamma_{\lambda s'}.\qquad(21)$$

Setting the partial derivatives of the above expression with respect to $a_{\lambda s}$ and $a_{\lambda s'}$ equal to zero, one obtains

$$a_{\lambda s} = (\tfrac{1}{2}\hbar)^{\frac{1}{2}}\gamma_{\lambda s}/(E_\lambda - E), \quad a_{\lambda s'}^* = (\tfrac{1}{2}\hbar)^{\frac{1}{2}}\gamma_{\lambda s'}/(E_\lambda - E).\qquad(22)$$

Inserting these results into the stationary expression, Eq. (21), one obtains

$$R_{ss'}^{(t)} = \sum_{\lambda=1}^{\xi} \frac{\gamma_{\lambda s}\gamma_{\lambda s'}}{E_\lambda - E},\qquad(23)$$

which is the same as the rigorous result up to the order of the trial function used. The variationally derived R matrix is also seen to be real and symmetric, as is the true R matrix, for all orders.

It is also interesting to note that the coefficients $a_{\lambda s}$ are equal to the expansion coefficients of the X_λ in the rigorous expansion of the wave function in the internal region. The variational procedure is thus seen simply to generate the rigorous expansion of the wave function in the internal region.

It is thus seen that one may derive directly a consistent finite-level formula for the R-matrix from a variation principle. It is also hoped that this work will lead to greater insight into the application of variation principles to continuum problems, in that the application presented is seen to lead to a process which converges to the true solution.