The value chosen for N was 20. These procedures were checked by applying them to series (A2) and (A3) which could be summed analytically. In addition, some internal checks were provided by the recurrence relations

$$\psi_1(k+1)-\psi_1(k)=1/k,$$
$$\psi_2(k+1)-\psi_2(k)=-1/k^2, \tag{A6}$$

which lead to the relations:

$$\sum_1^\infty \psi_1(k)P_k=\sum_1^\infty \psi_1(k)P_{k-1}+\gamma-\ln\frac{\csc^2\theta/2}{1+\csc\theta/2},$$

$$\sum_1^\infty \psi_1^2P_k=\sum_1^\infty \psi_1^2(k)P_{k-1}-\psi_1^2(1)-\sum_1^\infty\frac{P_k}{k^2}-2\sum_1^\infty\frac{\psi_1(k)P_k}{k^2},$$

$$\sum_1^\infty \psi_1(k)\psi_2(k)P_k=\sum_1^\infty \psi_1(k)\psi_2(k)P_{k-1}-\psi_1(1)\psi_2(1)+\sum_1^\infty\frac{\psi_1(k)P_k}{k^2}-\sum_1^\infty\frac{\psi_2(k)P_k}{k}+\sum_1^\infty\frac{P_k}{k^3},$$

$$\sum_1^\infty \psi_2P_k=\Sigma\,\psi_2P_{k-1}-\psi_2(1)+\Sigma\,P_k/k^2. \tag{A7}$$

Similar relations using the recurrence relations for the Legendre polynomials but were not found as useful except as used in (A4) and (A5). Another check was also provided by the asymptotic expansion for $\psi_2\to 1/k+1/2k^2+1/6k^3+\cdots$. It is estimated that the error in the computation of R is 0.1 percent.

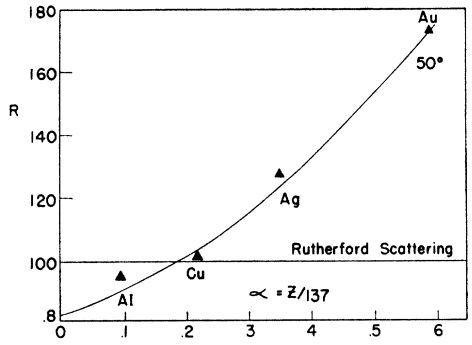

FIG. 5. Comparison of theory and experiment at electron energy of 2 Mev. The solid line is given by the theory. The triangles give the experimental points as obtained by Van de Graaff, Buechner *et al.*

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Variational Methods in Nuclear Collision Problems*

W. KOHN**
Department of Physics, Harvard University, Cambridge, Massachusetts
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Variational methods, similar to the Rayleigh-Ritz method for bound state calculations, are developed for the phase shifts and elements of the scattering matrix in nuclear collisions. Numerical applications to neutron-proton and neutron-deuteron scattering involving trial functions with undetermined coefficients are described. Another variational principle, for scattering amplitudes, is shown to lead to the Born approximations and a formula recently derived by Schwinger. It may also be used in conjunction with the method of undetermined coefficients.

I. INTRODUCTION

A GREAT deal of information about the nature of nuclear forces has been derived from a comparison of experimental and theoretical studies of simple nuclear systems.

The bound states of nuclei comprising up to four particles have been theoretically treated with considerable accuracy[1] and have yielded very important results. For nuclear collisions involving more than two particles, Breit and Wigner,[2] Wheeler,[3] Heisenberg,[4] and Wigner[5] have developed general, phenomenological theories. However, no very satisfactory scheme for treating such collisions in detail has so far been given. All calculations up to the present[6] are based on an approximation of the wave function by an

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** Parker Fellow, 1947–8.
[1] See, for example, W. Rarita and R. D. Present, Phys. Rev. **51**, 788 (1937); H. Margenau and D. T. Warren, Phys. Rev. **52**, 790 (1937).
[2] G. Breit and E. Wigner, Phys. Rev. **49**, 519 (1936).
[3] J. A. Wheeler, Phys. Rev. **52**, 1107 (1937).
[4] W. Heisenberg, Zeits. f. Physik **120**, 513 (1942).
[5] E. P. Wigner, Phys. Rev. **70**, 15 and 606 (1946).
[6] For example, L. Motz and J. Schwinger, Phys. Rev. **58**, 26 (1940); R. A. Buckingham and H. S. W. Massey, Proc. Roy. Soc. **179**, 123 (1941).

expression of the type

$$\Psi=\sum_i \varphi_i F_i, \tag{1.1}$$

where φ_i is the product of the internal wave functions of two colliding or separating nuclei[7] and F_i is the wave function of relative motion. The sum is taken over all pairs of nuclei whose formation is energetically possible and the signs adjusted in accordance with the exclusion principle. Wave functions of this so-called group structure type were first introduced by Wheeler.[3] While the function (1.1) has the correct symmetry and asymptotic behavior, one cannot expect it to describe too well the correct wave function in that part of the configuration space where the colliding nuclei interact, and it is just this region which determines the observable cross section.

To determine the best wave function of the group structure type, Wheeler employed a variational principle. Variational methods have also been applied by Hulthén[8] and Schwinger[9] to two-particle collisions.

The purpose of this paper is to propose variational methods, related to Hulthén's approach, which lead to stationary expressions for the observable scattering cross sections. In particular our methods lend themselves to a systematic treatment of composite collisions, which is not restricted to wave functions with group structure. The mathematical operations bear a considerable analogy to those of the Rayleigh-Ritz method for determining the binding energies of nuclei. The physical clue for this fact may be seen in the connection between binding energies and phase shifts which was pointed out by Heisenberg.[4] However, instead of attacking collision problems from this point of view, it will be simpler to investigate them independently of related bound states.

II. ONE-DIMENSIONAL PROBLEMS

In considering the collision of two particles, interacting by a short-range potential, one is led to the equation

$$\{d^2/dx^2+\kappa^2-V(x)\}u(x)=0, \tag{2.1}$$

for the partial wave of angular momentum 0; here κ is the wave number of relative motion and $V(x)$ the interaction potential. The wave function $u(x)$ has the following properties

$$u(0)=0, \tag{2.2}$$

$$x\to\infty: \quad u(x)\to A\sin\kappa x+B\cos\kappa x = A(\sin\kappa x+\tan\eta\cdot\cos\kappa x), \tag{2.3}$$

where A and B are some constants and the phase shift η is defined by $\tan\eta=B/A$.

Let the logarithmic derivative of $u(x)$ at $x=a$ be

$$L=u'(a)/u(a). \tag{2.4}$$

Then it is easily verified that u satisfies the equation

$$\int_0^a \{-(du/dx)^2+\kappa^2u^2-V(x)u^2\}dx + Lu^2(a)=0. \tag{2.5}$$

Furthermore, for a given value of L, κ^2 as calculated from (2.5) is stationary, if the trial functions, u_t, satisfy the condition (2.2). This fact is the basis of binding energy calculations. One can equally well regard (2.5) as providing a stationary expression for L, given the value of κ^2. This is the more natural approach in collision problems, in which the energy of the system is prescribed. If $x=a$ is beyond the range of interaction, $L=\kappa\cot(\kappa a+\eta)$, so that $\tan\eta$ and hence the scattering cross section, $\sigma=4\pi/\{\kappa^2(1+\cot^2\eta)\}$ can be calculated, once L is known.

To find an approximation for L from the stationary property of (2.5) we write our trial function in the form

$$u_t=c_1u_1+c_2u_2+\cdots c_nu_n, \tag{2.6}$$

where $u_i(0)=0$ and the unknown coefficients c_i are to be determined. Substituting (2.6) in (2.5), one is led to an equation of the form

$$Q\equiv\sum_{\substack{i=1\\j=1}}^{n} A_{ij}(\kappa^2)c_ic_j+L\Big(\sum_{i=1}^{n} c_iu_i(a)\Big)^2=0, \tag{2.7}$$

where we have indicated the dependence of the integrals A_{ij} on κ^2. We may, of course, assume that $A_{ij}=A_{ji}$.

The stationary property of (2.7) with respect to variations of the c_i now leads to the set of

[7] No systematic theory for nuclear collisions in which more than two end products are possible has yet been developed.

[8] L. Hulthén, Extrait, Dixième Congrès des Mathématiciens Scandinaves, Copenhague, 1946.

[9] Unpublished lectures. 1947.

equations,

$$\frac{\partial Q}{\partial c_i}=2\{\sum_{j=1}^{n} A_{ij}c_j+Lu_i(a)\cdot\sum_{j=1}^{n} u_j(a)c_j\}=0. \quad (2.8)$$

They are compatible only if the determinant of the coefficients of the c_i vanishes, i.e., if

$$\Delta\equiv|A_{ij}+Lu_i(a)\cdot u_j(a)|=0. \quad (2.9)$$

As the matrix $\|u_i(a)\cdot u_j(a)\|$ has rank 1, this is a *linear* equation for L and hence determines L uniquely.[10] This is in contrast to the usual secular determinants, whose degree in the unknown energy is as high as the number of trial functions. We shall refer to determinants of the character of Δ as collision determinants.

Another closely related variational principle can be derived as follows. Consider the expression

$$I\equiv\int_0^\infty u\{d^2/dx^2+\kappa^2-V(x)\}udx, \quad (2.10)$$

which vanishes if u is the correct solution of (2.1). Now let us consider its first variation, if the trial functions, $u_t=u+\delta u$ satisfy the conditions

$$u_t(0)=0,$$
$$x\to\infty: \quad u_t\to A\sin\kappa x+B_t\cos\kappa x. \quad (2.11)$$

Then, in virtue of the differential Eq. (2.1),

$$\delta I=\int_0^\infty (u\,d^2/dx^2\,\delta u-\delta u\,d^2/dx^2\,u)dx$$
$$=(u\,d/dx\,\delta u-\delta u\,d/dx\,u)_{x=\infty}=-\kappa A\delta B, \quad (2.12)$$

where $\delta B=B_t-B$. Hence,

$$\delta(I+\kappa AB)=0.^{11} \quad (2.13)$$

Since for the correct u, $I=0$, and $B=A\tan\eta$, the equation

$$I+\kappa AB_t=\kappa A^2\tan\eta, \quad (2.14)$$

is correct to the first order and hence serves as a variational principle for $\tan\eta$. As before, on using trial functions of the form (2.6) one is led to a collision determinant, Δ, which is linear in $\tan\eta$, so that the latter is uniquely determined by the compatibility equation, $\Delta=0$.

Numerical Illustrations

Using Eqs. (2.5) and (2.14), we have calculated scattering of neutrons by protons at zero energy. We have assumed the interaction

$$\left.\begin{aligned} V(x)&=-4.01435, \quad x\leqslant 1\\ &=0, \quad x>1\end{aligned}\right\} \quad (2.15)$$

(x measured in units of 2.80×10^{-13} cm), which gives the correct binding energy for the deuteron. The wave equation, in this case, is simply

$$d^2u/dx^2+V(x)u=0, \quad (2.16)$$

and can of course be solved exactly. For $x>1$, u has the form, $u=C(x+X)$, where X is the desired $\lim_{\kappa\to0}(\tan\eta/\kappa)$, in terms of which the scattering cross section is $4\pi X^2$. As trial functions we have used

$$u_t=\sum_1^n C_kx^k, \quad x\leqslant a(n=1,2,3). \quad (2.17)$$

Since (2.17) does not have the correct asymptotic form, required by (2.11), we have assumed that at $x=a$ it passes smoothly into a function of the form $u_t=Cx+D$.

Clearly, for a given n, a function of the type (2.17) can approximate the correct wave function better over a short than over a long interval, so that the best results are obtained with $a=1$ (see Table I).

III. THE SCATTERING AMPLITUDE

It is desirable to have methods for calculating the scattering amplitudes of the entire plane wave without having to determine, separately,

TABLE I. Approximations to $X=\lim_{\kappa\to0}\tan\eta/\kappa$; $X_{\text{exact}}=-2.080$; I.....by Eq. (2.5); II.....by Eq. (2.14).

a	c_1x		$c_1x+c_2x^2$		$c_1x+c_2x^2+c_3x^3$	
	I	II	I	II	I	II
1	−3.957	+1.338	−2.112	−2.126	−2.083	−2.084
2	+4.043	+1.338	−2.858	−4.039	−2.201	−2.206
3	+2.416	+1.338	−6.593	−51.606	−2.385	−2.520
4	+2.011	+1.338	968.870	+7.634	−2.936	−3.315

[10] This can also be made apparent by the transformation $d_1=\sum_1^n u_j(a)c_j$, $d_i=c_i$, $(i\neq1)$. Then Q has the form $Q=\sum_1^n B_{ij}d_id_j+Ld_1^2$, and the compatibility equation, $|B_{ij}+L\delta_{1i}\delta_{1j}|=0$, is evidently linear in L.

[11] L. Hulthén (see reference 8) has used an equivalent relation to determine $\tan\eta$, by restricting his trial functions by the condition $I=0$. This is a little complicated and leads to a quadratic equation for $\tan\eta$, only one of whose solutions is "good."

the phase shifts of each partial wave. This is usually accomplished by the use of successive Born approximations, i.e., by an iteration procedure. Another iteration method, giving more accurate results, has been developed by Schwinger.[9] We shall now derive a variational principle which serves as common basis of (a) Born approximations; (b) Schwinger's approximation; (c) The method of linear trial functions.

Let the wave equation of the problem be

$$\{\nabla^2+\kappa^2-V(\mathbf{r})\}\psi(\mathbf{r})=0, \tag{3.1}$$

where $\mathbf{r}$ is the usual relative position vector. We denote by ψ_1, ψ_2 the two solutions of (3.1) which correspond to plane waves incident along the vectors $\boldsymbol{\kappa}_1$ and $\boldsymbol{\kappa}_2$, respectively, ($|\boldsymbol{\kappa}_1|=|\boldsymbol{\kappa}_2|=\kappa$). They have the asymptotic form

$$\psi_i=\exp(i\boldsymbol{\kappa}_i\cdot\mathbf{r})+f(\boldsymbol{\kappa}_i,\boldsymbol{\kappa})\exp(i\kappa r)/r, \tag{3.2}$$

where $r=|\mathbf{r}|$ and $f(\boldsymbol{\kappa}_i,\boldsymbol{\kappa})$ is the scattering amplitude in the direction $\boldsymbol{\kappa}$ of a plane wave incident along $\boldsymbol{\kappa}_i$.

Next we define the bilinear form $I(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)$ as

$$I(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)=\int_0^\infty \psi_2\{\nabla^2+\kappa^2-V(\mathbf{r})\}\psi_1 d\mathbf{r}. \tag{3.3}$$

For the correct ψ_1, $I(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)=0$. Its first variation is

$$\delta I(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)=\int_S (\psi_2(\partial/\partial n)\delta\psi_1 - \delta\psi_1(\partial/\partial n)\psi_i)dS, \tag{3.4}$$

where S is a large sphere and $\partial/\partial n$ denotes differentiation along the outward normal. This follows immediately from an integration by parts.

If we admit only trial functions of the correct asymptotic form (3.2), but possibly false scattering amplitudes, $f_{t;i}(\boldsymbol{\kappa}_i,\boldsymbol{\kappa})$, then, asymptotically,

$$\delta\psi_i\to\delta f_i(\boldsymbol{\kappa}_i,\boldsymbol{\kappa})\exp(i\kappa r)/r. \tag{3.5}$$

Clearly only the plane wave part of ψ_2 contributes to the surface integral in (3.4), so that

$$\delta I(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)=\int_S \left\{\exp(i\boldsymbol{\kappa}_2\cdot\mathbf{r})\frac{\partial}{\partial n}\frac{\exp(i\kappa r)}{r} - \frac{\exp(i\kappa r)}{r}\frac{\partial}{\partial n}\exp(i\boldsymbol{\kappa}_2\cdot\mathbf{r})\right\}\cdot\delta f_1(\boldsymbol{\kappa}_1,\boldsymbol{\kappa})dS. \tag{3.6}$$

Dirac[12] has shown that the factor multiplying $\delta f_1(\boldsymbol{\kappa}_1,\boldsymbol{\kappa})$ has a δ-function like character for large values of r, so that the integration simply gives $-4\pi\delta f_1(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)$. Hence, corresponding to (2.14) we find

$$I(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)+4\pi f_{t;1}(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)=4\pi f(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2), \tag{3.7}$$

as a stationary expression for $f(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)$ relative to independent variations of ψ_1 and ψ_2, subject to the conditions (3.5).

More generally, if we admit trial functions of the asymptotic form

$$\psi_{t;i}\to A_t\left\{\exp(i\boldsymbol{\kappa}_i\cdot\mathbf{r})+f_{t;i}(\boldsymbol{\kappa}_i,\boldsymbol{\kappa})\frac{\exp(i\kappa r)}{r}\right\}, \tag{3.8}$$

(3.7) is replaced by the homogeneous equation

$$I(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)+4\pi A_t^2 f_{t;1}(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)=4\pi A_t^2 f(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2), \tag{3.9}$$

where $I(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2)$ is defined as before, Eq. (3.3).

Born Approximations

The simplest admissible trial functions are $\psi_i=\exp(i\boldsymbol{\kappa}_i\cdot\mathbf{r})$ which, by (3.7), directly yield the first Born approximation,

$$-\int \exp(i\boldsymbol{\kappa}_2\cdot\mathbf{r})\,V(\mathbf{r})\,\exp(i\boldsymbol{\kappa}_1\cdot\mathbf{r}) = 4\pi f(\boldsymbol{\kappa}_1,-\boldsymbol{\kappa}_2). \tag{3.10}$$

The second Born approximation is obtained by using either

$$\psi_1=\exp(i\boldsymbol{\kappa}_1\cdot\mathbf{r});\qquad \psi_2=\exp(i\boldsymbol{\kappa}_2\cdot\mathbf{r}) - \int(\exp(i\kappa|\mathbf{r}-\mathbf{r}'|)/4\pi|\mathbf{r}-\mathbf{r}'|) \times V(\mathbf{r}')\exp(i\boldsymbol{\kappa}_2\cdot\mathbf{r}')d\mathbf{r}', \tag{3.11}$$

or

$$\psi_1=\exp(i\boldsymbol{\kappa}_1\cdot\mathbf{r}) - \int(\exp(i\kappa|\mathbf{r}-\mathbf{r}'|))/(4\pi|\mathbf{r}-\mathbf{r}'|) \times V(\mathbf{r}')\exp(i\boldsymbol{\kappa}_1\cdot\mathbf{r}')d\mathbf{r}'; \tag{3.11'}$$

$\psi_2=\exp(i\boldsymbol{\kappa}_2\cdot\mathbf{r})$.[13]

[12] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Clarendon Press, Oxford, 1947), third edition, p. 191.

[13] The symmetry with respect to the functional forms of ψ_1 and ψ_2 is a general property of this method.

Higher Born approximations are obtained in a similar way.

Schwinger's Approximation

The correct ψ_1 satisfies the integral equation

$$\psi_1(\mathbf{r}) = \exp(i\boldsymbol{\kappa}_1\cdot\mathbf{r}) - \int (\exp(i\kappa|\mathbf{r}-\mathbf{r}'|)/4\pi|\mathbf{r}-\mathbf{r}'|) \times V(\mathbf{r}')\psi_1(\mathbf{r}')d\mathbf{r}'. \quad (3.12)$$

Using the well-known equation

$$f(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2) = -1/4\pi \int \exp(i\boldsymbol{\kappa}_2\cdot\mathbf{r}') \times V(\mathbf{r}')\psi_1(\mathbf{r}')d\mathbf{r}', \quad (3.13)$$

we can rewrite (3.12) in the homogeneous form

$$\psi_1(\mathbf{r}) = -\int G(\mathbf{r},\mathbf{r}')\,V(\mathbf{r}')\psi_1(\mathbf{r}')d\mathbf{r}, \quad (3.14)$$

where

$$G(\mathbf{r},\mathbf{r}') = 1/(4\pi f(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2)) \times \exp(i\boldsymbol{\kappa}_1\cdot\mathbf{r})\cdot\exp(i\boldsymbol{\kappa}_2\cdot\mathbf{r}') + \exp(i\kappa|\mathbf{r}-\mathbf{r}'|)/(4\pi|\mathbf{r}-\mathbf{r}'|). \quad (3.15)$$

Equation (3.14) has the property that regardless of what function is used for ψ_1 in the right-hand side, the left-hand side, in virtue of (3.15), is a wave function whose scattering amplitude from $\boldsymbol{\kappa}_1$ to $-\boldsymbol{\kappa}_2$ is $f(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2)$.

In (3.8) we now use some trial function ψ_2 and a function ψ_1 of the form

$$\psi_1 = -\int G(\mathbf{r},\mathbf{r}')\,V(\mathbf{r}')\varphi_1(\mathbf{r}')d\mathbf{r}'. \quad (3.16)$$

Since now $f_{l;1}(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2) = f_1(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2)$, (3.9) becomes simply $I(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2) = 0$, which when written out in full is

$$0 = \int \psi_2(\mathbf{r})\,V(\mathbf{r})\varphi_1(\mathbf{r})d\mathbf{r} + \int\int \psi_2(\mathbf{r})\,V(\mathbf{r}) \times (\exp(i\kappa|\mathbf{r}-\mathbf{r}'|))/(4\pi|\mathbf{r}-\mathbf{r}'|) \times V(\mathbf{r}')\varphi_1(\mathbf{r}')d\mathbf{r}d\mathbf{r}' + \frac{1}{4\pi f(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2)} \times \int \psi_2(\mathbf{r})\,V(\mathbf{r})\exp(i\boldsymbol{\kappa}_1\cdot\mathbf{r})d\mathbf{r} \times \int \varphi_1(\mathbf{r})\,V(\mathbf{r})\exp(i\boldsymbol{\kappa}_2\cdot\mathbf{r})d\mathbf{r}. \quad (3.17)$$

This is Schwinger's variational principle for the determination of $f(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2)$.

Linear Trial Functions

For simplicity, we use the same functional form for ψ_1 and ψ_2 and write

$$\psi_i = c_1\exp(i\boldsymbol{\kappa}_i\cdot\mathbf{r}) + \sum_{l=2}^{n} c_l u_{i;l}, \quad i=1,2, \quad (3.18)$$

where $u_{1;l}$ and $u_{2;l}$ differ only by a rotation of the coordinates and have the asymptotic form

$$u_{i;l} \to f_l(\boldsymbol{\kappa}_i, \boldsymbol{\kappa})(\exp(i\kappa r))/(r). \quad (3.19)$$

Then

$$f_l^{(1)}(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2) = 1/c_1 \sum_{l=2}^{n} c_l f_l(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2), \quad (3.20)$$

so that (3.8) gives

$$I(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2) + 4\pi c_1 \sum_{l=2}^{n} c_l f_l(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2) = 4\pi c_1^2 f(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2). \quad (3.21)$$

As in the one-dimensional case, $f(\boldsymbol{\kappa}_1, -\boldsymbol{\kappa}_2)$ is uniquely determined by the vanishing of the collision determinant corresponding to (3.21).

IV. COMPOSITE COLLISIONS: THEORY[14]

We consider processes of the following kind: A number of nucleons, divided into alternative pairs, collide within a region of interaction and then re-emerge into the asymptotic region, grouped again into pairs.[15]

Let φ_i be the normalized product of the internal wave functions of the nuclei constituting the pair i, and let F_i be the wave function of relative motion when they are apart. Then the function

$$\Phi_i = \varphi_i F_i, \quad (4.1)$$

will be called a mode of collision. On a hypersurface, S, separating the region of interaction from the external region, the wave function, Ψ, of the entire system has the form

$$\Psi = \sum_i \Phi_i. \quad (4.2)$$

[14] Many of the mathematical operations of this section are similar to those employed and explained by E. P. Wigner (see reference 5).

[15] It is assumed that disintegrations into three or more particles cannot occur and that at least one constituent of each pair is electrically neutral.

Let us note that, even barring accidental degeneracies, the proper functions of the Hamiltonian, H, are highly degenerate for two reasons:

(a) The spatial orientation of Ψ is arbitrary.
(b) The amplitudes of the incoming waves of the different modes are arbitrary.

A degeneracy of the type (a) was made use of in Section III to deduce a variational principle for the scattering amplitude $f(\kappa_1, \kappa_2)$ from one asymptotic state into another. In precisely the same way we shall in this section develop a variational principle for the scattering amplitude, into the mode Φ_j of nucleons colliding in the mode Φ_i. To avoid complications we remove the degeneracy (a) by considering only such functions Ψ which belong to the same proper values of the total angular momentum, J, and its z component, J_z. With this restriction the modes satisfy the orthogonality relations

$$\int_S \Phi_i \Phi_j^* dS = 0, \quad i \neq j. \tag{4.3}$$

For if the modes Φ_i and Φ_j describe different groupings of nucleons, they exist on different portions of S and hence (4.3) is satisfied; while if they describe the same groupings, the internal wave functions of the nuclei must be orthogonal so that (4.3) follows in this case also.

The Elements of the Scattering Matrix

Let $\Psi^{(1)}$ and $\Psi^{(2)}$ be two wave functions of the relative coordinates of the nucleons, belonging to the same proper values of H, J, and J_z but differing in the amplitudes of their modes. We write their asymptotic form on the surface S as

$$\begin{aligned}\Psi^{(\mu)} &= \sum_i \Phi_i^{(\mu)} \\ &= \sum_i \varphi_i (S_i/c_i)(\alpha_i^{(\mu)} \exp(-i\kappa_i r_i)/r_i \\ &\qquad - \beta_i^{(\mu)} \exp(i\kappa_i r_i)/r_i), \end{aligned} \tag{4.4}$$

where we have decomposed the function of relative motion into its angular and radial parts. r_i is the separation of the centers of gravity of the nuclei of the mode Φ_i; κ_i is the wave number and S_i the normalized angular wave function of relative motion; c_i is a constant chosen so that $|\alpha_i^{(\mu)}|^2$ represents the probability flux resulting from the mode Φ_i into the interior of S. It has the value $c_i = (2E_i/M_i)^{\frac{1}{2}} = (\hbar\kappa_i/M_i)^{\frac{1}{2}}$, where E_i is the energy of relative motion and M_i the reduced mass of the two nuclei. The sum in (4.4) is taken over all possible pairs of nuclei.

Before developing variational principles for the elements of the scattering matrix, let us note that in the case of a continuum of degenerate states the symbol δ for the first variation must be carefully defined. Thus, let Ψ_t be a trial function of the form (4.4), but with possibly incorrect α_i, β_i, and φ_i; then $\delta\Psi = \Psi_t - \Psi$, where Ψ is *some* neighboring correct function. For example, we may choose Ψ to agree with Ψ_t in the values of

(a) the amplitudes, α_i, of the incoming waves;
(b) the amplitudes, β_i, of the outgoing waves.

Consider now the integral

$$I_{12} = \int_V \Psi^{(1)*}(H-E)\Psi^{(2)} d\tau, \tag{4.5}$$

where V is the region enclosed by S, and H and E are the total Hamiltonian and energy, after the motion of the center of gravity has been separated out. We now define $\delta\Psi^{(1)}$ according to (b) and $\delta\Psi^{(2)}$ according to (a), so that $\beta_{i,t}^{(1)} = \beta_i^{(1)}$ and $\alpha_{i,t}^{(2)} = \alpha_i^{(2)}$. δI_{12} is the corresponding variation of I_{12}. It can be evaluated in terms of the α_i and β_i by transforming the volume integral arising from (4.5) to an integral over the hypersurface S by Green's theorem (cp. (2.12)) and by making use of the orthogonality relations (4.3). (For details see reference 5.) In this way one obtains

$$\delta I_{12} = -i\hbar \sum \beta_i^{(1)*} \cdot \delta\beta_i^{(2)}. \tag{4.6}$$

It should be noted that, to the first order, errors of the internal wave functions of the colliding nuclei do not appear. For the correct $\Psi^{(2)}$, $I_{12} = 0$, and hence the equation

$$I_{12} + i\hbar \sum_i \beta_i^{(1)*} \cdot \beta_{i,t}^{(2)} = i\hbar \sum_i \beta_i^{(1)*} \cdot \beta_i^{(2)}, \tag{4.7}$$

is correct to the first order.

We now introduce the scattering matrix, S_{ij}, belonging to the energy and total angular momentum under consideration, which is defined by the equations

$$\beta_i^{(\mu)} = \sum_j S_{ij} \alpha_j^{(\mu)}, \tag{4.8}$$

and embodies all observable scattering properties. Then (4.7) may be written as

$$I_{12}+i\hbar\sum_i \beta_i^{(1)*}\beta_{i,t}^{(2)}=i\hbar\sum_{i,j}\beta_i^{(1)*}S_{ij}\alpha_j^{(2)}, \quad (4.9)$$

where all quantities, except the elements S_{ij}, are determined by the trial functions. This is a homogeneous variational principle for the matrix elements S_{ij}, allowing directly the application of the method of linear trial functions. For example, to find the element S_{56} one would choose trial functions with $\beta_i^{(1)}=c^{(1)}\delta_{i5}$ and $\alpha_j^{(2)}=c^{(2)}\delta_{i6}$ in which case the right-hand side of (4.9) reduces to $i\hbar c^{(1)*}c^{(2)}S_{56}$; the stationary property of S_{56} relative to variations of the undetermined coefficients uniquely determines its value with an error of the second order in $\delta\Psi^{(\mu)}$. The wave functions can then be found in the usual way correct to the first order.

The Proper Phases of the Scattering Matrix

If the system of nucleons can group itself into n modes, the matrix S_{ij} has rank n, and n proper values, σ_m, satisfying the equations

$$\beta_i^{(\mu m)}=\sum_i S_{ij}\alpha_i^{(\mu m)}=\sigma_m\alpha_i^{(\mu m)}, \qquad m=1, 2, \cdots n; \quad (4.10)$$

the $\alpha_i^{(\mu m)}$ and $\beta_i^{(\mu m)}$ are the amplitudes of the proper wave functions. Because of the unitary property of the matrix S_{ij}, the σ_m have unit magnitude and hence can be written as $\sigma_m=\exp(2i\eta_m)$, where the η_m are referred to as proper phases of S_{ij}. The corresponding wave functions have, asymptotically, the form of standing waves.

Schwinger[9] has suggested the use of proper phases in collision problems, and has shown that the total cross section in neutron-proton scattering with tensor forces is expressible in terms of these phases.

To find a variational principle for the η_m, consider the expression

$$I=\int_V \Psi^*(H-E)\Psi d\tau, \quad (4.11)$$

where Ψ is a proper function of S_{ij} (corresponding to one of the σ_m), with the asymptotic form

$$\Psi\rightarrow\sum \varphi_i S_i(A_i j_{l_i}+B_i n_{l_i}); \quad (4.12)$$

the j_{l_i} and n_{l_i} are the spherical Bessel and Neumann functions of the argument $\kappa_i r_i$ and of the order l_i, where l_i is the relative angular momentum of the nuclei in the mode i.

We assume now that our trial functions have the correct asymptotic form, (4.12), although possibly the internal functions φ_i and the coefficients A_i and B_i may have first-order errors. Thus, asymptotically,

$$\delta\Psi=\sum \varphi_i S_i(\delta A_i j_{l_i}+\delta B_i n_{l_i}) +\sum \delta\varphi_i S_i(A_i j_{l_i}+B_i n_{l_i}). \quad (4.13)$$

In evaluating δI, we use the fact that

$$(H-E)\Psi=0,$$

which gives

$$\delta I=\int_V \{\Psi^* T\delta\Psi-\delta\Psi T\Psi^*\}d\tau, \quad (4.14)$$

where T is the kinetic energy operator. This may be converted to a surface integral in which the asymptotic forms (4.12) and (4.13) can be used to give, after some straightforward calculation,

$$\delta I=-\sum_i (\hbar^2)/(2M_i\kappa_i)\{A_i\delta B_i-B_i\delta A_i\} =\sum_i (\hbar^2)/(2M_i\kappa_i)\{\delta(A_iB_i) -(B_i)/(A_i)\delta(A_i^2)\}. \quad (4.15)$$

Since for a proper function all ratios B_i/A_i equal $-\tan\eta_m$, it follows that

$$\delta\{I+\sum_i (\hbar^2)/(2M_i\kappa_i) \times(A_iB_i+\tan\eta_m A_i^2)\}=0, \quad (4.16)$$

where $\tan\eta_m$ is considered fixed at its correct value. As the curly bracket vanishes for a correct Ψ, the equation

$$I+\sum_i (\hbar^2)/(2M_i\kappa_i)A_{i,t}B_{i,t} =-\tan\eta_m\sum_i (\hbar^2)/(2M_i\kappa_i)A_{i,t}^2, \quad (4.17)$$

provides a stationary expression for $\tan\eta_m$. The collision determinant, Δ, arising from the method of linear trial functions is of the nth degree in the unknown $\tan\eta_m$ corresponding to the sum of n squares multiplying it.[16] The n solutions of the

[16] Certain modes differ only by interchanges of identical particles. Hence their amplitudes must agree within a factor of ±1, determined by the Pauli principle. This al-

equation $\Delta=0$ are variational approximations to the tangents of the n proper phases, η_m. The proper wave functions are then determined as usual.

To determine the cross sections of some given physical process (e.g., only certain modes incoming) one must, in general, take suitable linear combinations of the proper functions of S_{ij}, in each of which every mode is both incoming and outgoing with a certain amplitude. However, since the proper functions involve first-order errors even asymptotically (the phase shifts are determined to the second order, but the relative amplitudes of the modes only to the first order) the cross sections so calculated will also have first-order errors. Exceptions from this rule are neutron-deuteron and proton-deuteron scattering, without tensor forces (Section V), where the relative amplitudes are known exactly from symmetry considerations, so that the method of proper phases gives the physical scattering cross section correct to the second order.

V. COMPOSITE COLLISIONS: NUMERICAL APPLICATIONS

The theory developed in the preceding section has been applied to two simple systems: The neutron-proton system with the inclusion of tensor forces and the neutron-deuteron system, at low energies, assuming central forces. The first calculation is simple and could be checked against a numerical integration by Schwinger. The second calculation demands the use of a great number of trial functions, because of the three-dimensional character of the wave function. Only preliminary results have been obtained in this case.

TABLE II. $^3S_1+^3D_1$ scattering with tensor forces.

Trial functions	Uncoupled $\tan\eta_S$	Uncoupled $\tan\eta_D$	Coupled $\tan\eta_1$	Coupled $\tan\eta_2$
$u=c_1r+c_2r^2$, $w=d_1r^3$	6.9850	−0.3199	+6.986	−0.0003
$u=c_1r+c_2r^2$, $w=d_1r^3+d_2r^4$	6.9850	−0.3070	−1.525	−0.0002
$u=c_1r+c_2r^2+c_3r^3$, $w=d_1r^3+d_2r^4$	9.1398	−0.3070	−1.425	−0.0002
Correct functions	9.2314	−0.3069	−1.435[9]	0.0000[9]

lows one to reduce the number of squared unknowns multiplying $\tan\eta_m$ in (4.17) and hence the degree of the collision determinant.

Neutron-Proton Scattering with Tensor Forces

At low energies the scattering is mainly due to the $^3S_1+^3D_1$ part of the wave function. Rarita and Schwinger[17] have shown that for this partial wave the Schroedinger equation leads to two coupled equations,

$$\begin{aligned}((d^2)/(dr^2)+\kappa^2)u+\lambda(fu+gw)=0,\\ ((d^2)/(dr^2)-6/r^2+\kappa^2)w+\lambda(gu+hw)=0,\end{aligned}\tag{5.1}$$

where $u(r)$ and $w(r)$ are the radial functions of the S and D wave, respectively. Following reference 17 we set

$$\begin{aligned}&\lambda=2.62828,\\ &f(r)=-1, \quad r\leqslant 1\\ &\quad\ =0, \quad\ r>1,\\ &g(r)=2.19203f(r); \quad h(r)=4.10000f(r).\end{aligned}\tag{5.2}$$

It is simpler to base our variational procedure directly on Eqs. (5.1) rather than go back to the three-dimensional Schroedinger equation. Thus we define

$$I=\int_0^\infty \{u[(d^2/dr^2+\kappa^2)u+\lambda(fu+gw)]$$
$$+w[(d^2/dr^2+\kappa^2-b/r^2)w+\lambda(gu+hw)]\}dr. \tag{5.3}$$

If we use trial functions with the asymptotic form

$$\begin{aligned}u&=r[A_{S,t}j_0(\kappa r)+B_{S,t}n_0(\kappa r)],\\ w&=r[A_{D,t}j_2(\kappa r)+B_{D,t}n_2(\kappa r)],\end{aligned}\tag{5.4}$$

we find the following variational principle for $\tan\eta_m$:

$$I-1/\kappa(A_{S,t}B_{S,t}+A_{D,t}B_{D,t})$$
$$=1/\kappa(A_{S,t}^2+A_{D,t}^2)\tan\eta_m. \tag{5.5}$$

We have used the trial functions

$$\left.\begin{aligned}u_p&=\sum_1^p c_kr^k, \qquad p=1,2,3\\ w_q&=\sum_1^q d_kr^{k+2}, \quad q=1,2\end{aligned}\right\} r\leqslant 1, \tag{5.6}$$

and the expressions (5.4) for $r>1$. $A_{S,t}$, $B_{S,t}$, $A_{D,t}$, $B_{D,t}$ were determined from the conditions that at $r=1$, the functions (5.6) pass smoothly into the free particle wave functions (5.4).

[17] W. Rarita and J. Schwinger, Phys. Rev. **59**, 436 (1941).

As checks on our calculation we have at each stage computed by the variational method the S and D phase shifts when tensor forces are absent and compared the results with the exact values which are easily obtained for the uncoupled states. The results of our calculations are collected in Table II.

It is seen that the last pair of trial functions gives good agreement with Schwinger's numerical integration, given in the last row.

Neutron-Deuteron Scattering

We have made an exploratory calculation of S scattering in the limit of vanishing neutron energy. For the interaction between the nucleons i and j we have assumed a Wigner potential

$$V_{ij} = -V_0 \exp(-(r_{ij})^2/b^2), \tag{5.7}$$

where $V_0 = 72.00$ mc^2, r_{ij} is the distance between the nucleons, and $b = 2.24\times10^{-13}$ cm. These constants give the correct deuteron binding energy.

Let us now introduce the vectors $\boldsymbol{\rho}_1$ and $\mathbf{r}_1$ from the proton, 3, to the neutron, 2, and from the center of mass of 2 and 3 to the neutron, 1, respectively. (See Fig. 1.) Further, if P_{12} denotes interchange of the neutrons 1 and 2 we define $\boldsymbol{\rho}_2 = P_{12}\boldsymbol{\rho}_1$ and $\mathbf{r}_2 = P_{12}\mathbf{r}_1$.

As trial function we have used

$$\Psi_t = [\varphi_t(\rho_1)\chi_1]F_t(r_1) - [\varphi_t(\rho_2)\chi_2]F_t(r_2), \tag{5.8}$$

where

$$\begin{aligned}
&\varphi_t(\rho) = (0.0904468)\exp(-(0.0637755)\rho^2);\\
&F_t(r) = c_0 + c_2r^2 + c_4r^4, \quad r < 8.4\times10^{-13}\text{ cm};\\
&\chi_1 = \chi_2 = \alpha(1)\alpha(2)\alpha(3)\\
&\qquad\qquad \text{for quartet scattering;}\\
&\chi_1 = P_{12}\chi_2 = 6^{-\frac{1}{2}}[\alpha(1)\alpha(2)\beta(3)\\
&\qquad +\alpha(1)\beta(2)\alpha(3) - 2\beta(1)\alpha(2)\alpha(3)]\\
&\qquad\qquad \text{for doublet scattering.}
\end{aligned} \tag{5.9}$$

The function (5.8) has group structure, for simplicity, but our methods are not restricted to this type of trial function (see Section VI). Our polynomial expression for F_t has the wrong asymptotic form. Hence at some distance $r = a$ it was assumed to pass smoothly into the correct asymptotic form $C + D/r$. We found that the smallest a including the region of interaction was approximately 8.4×10^{-13} cm.

In order to eliminate meaningless contributions to I which come from the error of the trial function for the deuteron wave function (see (5.9)), we have replaced E in the expression (4.5) for I by the expectation value of the deuteron Hamiltonian in the deuteron *trial* function. Because of the stationary nature of the deuteron binding energy, the change is of the second order and hence theoretically legitimate.

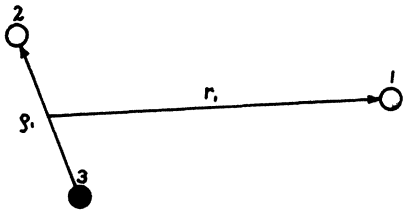

FIG. 1.

We have calculated by the formula (4.17) the quantities $X = \lim_{\kappa\to0} \tan\eta/\kappa$, where κ is the wave number and η the phase shift of the incident neutron, for quartet and doublet scattering. If we denote these by X_q and X_d, respectively, the total cross section in the limit of zero collision energy is

$$\sigma = 4\pi(\tfrac{2}{3}X_q^2 + \tfrac{1}{3}X_d^2). \tag{5.10}$$

The values obtained were $X_q = 5.12\times10^{-13}$ cm and $X_d = 4.20\times10^{-13}$ cm. In the case of X_d it appears that inclusion of more terms in F_t may appreciably alter the result. The cross section corresponding to our calculated values of X_q and X_d is 2.9 barns. This compares reasonably well with the recently published experimental value of 3.3 ± 0.2 barns.[18]

No great significance is claimed for the result of this calculation which was carried out primarily to provide a rough test of our method. It should be extended by using more elaborate trial functions as well as different types of interaction.

VI. DISCUSSION

The methods which we have described bear a strong analogy to the Rayleigh-Ritz method for the determination of the binding energies of bound nuclei. The chief new features, in collision problems, are the following.

(a) The trial functions must, asymptotically, become sums of products, as do the actual wave functions (see (4.4) or (4.8)).

[18] Rainwater, Havens, Jr., Dunning, and Wu, Phys. Rev. **73**, 733 (1948).

(b) In the determination of elements of the scattering matrix the integral I is bilinear (see, for instance, (4.5)), involving two different trial functions, as compared to the quadratic forms encountered in binding energy calculations. This is a reflection of the degeneracy of collision functions, corresponding to the arbitrariness of the amplitudes of the incident waves.

(c) The scattering properties are determined as solution of a determinantal equation, whose degree in the unknown is determined by the problem itself and not by the number of trial functions, as in bound state problems. For elements of the scattering matrix this degree is 1; for the tangents of the proper phase shifts it equals the number of physically different modes into which the system can split.

In numerical calculations one requires matrix elements of the Hamiltonian and total energy just as in binding energy problems. Thus the labor involved is approximately the same except for the somewhat more complicated trial functions in collision calculations. Here, to assure convergence to the correct answer, one must use trial functions of the form

$$\Psi_t=\sum_i \varphi_{i;t}(a_i f_i+b_i g_i)S_i/c_i+\sum_n c_n\psi_n, \quad (6.1)$$

where $f_i\rightarrow\sin\kappa_i r_i/r_i$, $g_i\rightarrow\cos\kappa_i r_i/r_i$, the $\varphi_{i;t}$ are trial functions for the internal wave functions of the colliding nuclei and the ψ_n are a complete set of functions vanishing rapidly at infinity. The first sum is required to describe the asymptotic behavior, the second to describe the region of interaction. In binding energy calculations only the second sum is required.

On the other hand, the necessity of solving high order determinantal equations does not arise in reasonably simple collision problems, which is a simplification over binding energy calculations.

In view of the great theoretical interest attaching to the scattering of light nuclei, more extensive calculations along the indicated lines, perhaps with the aid of electronic computing machines, would appear desirable.

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