A Variational Calculation on the $n$-$d$ System

---An Extended Resonating-Group Method---

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A variational principle of Kohn-type is derived for elastic $n$-$d$ scattering below and above deuteron-breakup in the framework of the Faddeev equations. The two-body central local potential is assumed. Applying this principle, we evaluate the $s$-wave phase shifts of elastic $n$-$d$ scattering and the triton binding energy. Introducing a pair correlation function in the trial function, we obtain equations of an extended resonating-group structure. As an illustration, these equations are solved for a Gaussian potential. It is found that for incident energies below 15 MeV, the results of the usual resonating-group model are much improved in the doublet state and the empirical effective range formula for this state is well reproduced. The interaction mechanisms of low-energy $n$-$d$ scattering are also visualized in a simple manner.

§ 1. Introduction

As a typical nuclear three-body problem, the properties of triton and $n$-$d$ scattering have been extensively studied. The main theoretical interest lies in studying to what extent we can explain the three-nucleon system with two-nucleon interactions. This implies, for one thing, to discriminate among various two-nucleon potentials which can reproduce the two-nucleon data equally well and, for another thing, to see whether or not we can finally understand the three-nucleon system by the two-nucleon potential.

The $n$-$d$ quartet scattering is explained satisfactorily by various approaches, not depending on potential shapes; in the quartet state, two neutrons cannot be close to each other by the Pauli principle. For the doublet state, all existing calculations using realistic two-nucleon potentials give the triton binding energy of about 6 to 7.5 MeV which are appreciably smaller than the observed one, 8.48 MeV, and give the doublet scattering length of about 1 to 2.5 fm which are appreciably larger than the observed one, 0.1 to 0.7 fm. On the other hand, calculations using effective central local two-nucleon potentials without repulsive core show appreciable overbinding of triton and give the doublet scattering length smaller than the observed one. Inclusion of repulsive core improves the situation.

The striking behavior of the observed values of $k \cot \delta$ in the doublet state near threshold has been studied by several authors. Calculations using central square well without repulsive core reproduce excellently the threshold behavior,
A Variational Calculation on the n-d System

but the calculated values of $k \cot \theta$ deviate from the experimental ones beyond deuteron-breakup. Calculations using dispersion relations\(^6\) show that the threshold behavior is qualitatively reproduced by the interference between long-range proton exchange and short-range background forces, provided that the value of the doublet scattering length is known.

Now, from these investigations it appears that any detailed calculation using realistic potentials has not been done yet, attempting to reproduce systematically the observed values of $k \cot \theta$ in the doublet state above as well as below deuteron-breakup and the triton binding energy. Since such a calculation using realistic potentials is of course very difficult in practice, the use of effective central local potentials in studying the n-d system at low energies still has its meaning as preparation for future calculations with more realistic potentials.

The purpose of this paper is to perform a variational calculation on the n-d system at low energies with effective central local potentials, to determine approximate wave functions in configuration space and to elucidate quantitatively the interaction mechanisms in a physically transparent way. Our method leads to a resonating-group model\(^1\) improved so as to take account of the distortion effect of the wave function induced directly by the nucleon-nucleon interaction in a form of pair correlation functions.

In § 2, a variational principle of Kohn-type\(^9\) is derived for elastic n-d scattering in the framework of the Faddeev equations.\(^10\) In § 3, this principle is applied to the evaluation of the s-wave phase shifts of elastic n-d scattering and the triton binding energy. In § 4, we make as an illustration a numerical evaluation using a Gaussian potential while § 5 is devoted to discussion of the results.

§ 2. Derivation of variational principle

A preliminary derivation is given in Ref. 15) and the final form is essentially the same as given there. We present here a more compact and rigorous way of derivation based on the Faddeev formalism.

In Verde's notation,\(^10\) the total wave functions for the n-d system are given by

\[ \Psi_{1A} = \psi' \chi'' \chi' \chi'' \quad \text{for Quartet} \]

and

\[ \Psi_{1B} = \frac{1}{2} (\psi^+ + \psi^-) \chi' \chi'' + \frac{1}{2} (\psi^+ - \psi^-) \chi' \chi'' \]

\[ - \frac{1}{2} (\psi^+ + \psi^-) \chi' \chi'' + \frac{1}{2} (\psi^+ - \psi^-) \chi' \chi'' \quad \text{for Doublet}. \]

Following Sitenko and Kharchenko,\(^17\) we decompose $\Psi_2$ into the Faddeev channel functions as follows:
where we label the coordinates as shown in Fig. 1. Then, we have the Faddeev equations

\[(T + U_i - E) \psi^{(i)} = - U_i [\psi^{(j)} + \psi^{(k)}], \tag{2.4}\]

where \(i, j\) and \(k\) are the permutations of 1, 2 and 3, \(T\) the total kinetic energy operator, \(E\) the total energy and \(U_i\) the potential between nucleons \(j\) and \(k\). Combining Eqs. (2.4), we have the Schrödinger equation:

\[(T + U_1 + U_2 + U_3) \Psi_s = E \Psi_s. \tag{2.5}\]

For \(n-d\) scattering, the incident wave is represented by

\[\Phi_1 = e^{i K_i \cdot r_i} \phi(r_i) \times \begin{cases} \chi \chi' & \text{for Quartet,} \\ \zeta \zeta' & \text{for Doublet,} \end{cases} \tag{2.6a}\]

where \(K_i\) is the c.m. momentum of the incident neutron and \(\phi\) the deuteron ground state function. It is an essential point of the Faddeev decomposition (2.3) that the channel function \(\psi^{(i)}\) involves only the plane wave \(e^{i K_i \cdot r_i} \phi(r_i)\), whereas \(\Psi_s\) involves also the plane waves \(e^{i K_i \cdot r_i} \phi(r_i)\) and \(e^{i K_i \cdot r_i} \phi(r_i)\).

The amplitude of elastically scattered wave is then given by

\[f(\theta) = \frac{1}{3\pi} \left[ \bar{\Phi}_1 (T + U_1 - E) \Psi_s d\tau \right], \tag{2.7}\]

where

\[d\tau = d^3 R_1 d^3 r_1 \tag{2.8}\]

and \(\bar{\Phi}_1\) is the same as \(\Phi_1\) except that \(K_i\) is replaced by \(-K_i, K_f\) being the c.m. momentum of the elastically scattered neutron.

Now, we consider a trial wave function \(\Psi_t\) for \(\Psi_s\) and put

\[\Psi_s = \Psi_t - \partial \Psi, \tag{2.9}\]

\(\partial \Psi\) being the error in the wave function. We also define the adjoints of them as \(\bar{\Psi}_t, \bar{\Psi}_s\) and \(\bar{\Psi}\), for which \(K_i\) is replaced by \(-K_i\) in the incident wave. We
A Variational Calculation on the n-d System

then have

\[ f(\theta) = f_1(\theta) - \frac{1}{3\pi} \int \mathbf{\phi}_1(T + U_1 - E) \partial \mathbf{F} \, d\tau \]  

(2.10)

with

\[ f_1(\theta) = \frac{1}{3\pi} \int \mathbf{\phi}_1(T + U_1 - E) \mathbf{F} \, d\tau . \]  

(2.11)

We put the second term of Eq. (2.10) into the following form:

\[ \int \mathbf{\phi}_1(T + U_1 - E) \partial \mathbf{F} \, d\tau = \int [\mathbf{\phi}_1 - \mathbf{\phi}_1^{(w)}] (T + U_1 - E) \partial \mathbf{F} \, d\tau \]

\[ + \int \mathbf{\phi}_1^{(w)} (T + U_1 - E) \partial \mathbf{F} \, d\tau , \]  

(2.12)

where \( \mathbf{\phi}_1^{(w)} \) is the component of the Faddeev decomposition of \( \mathbf{\Pi} \), namely

\[ \mathbf{\Pi}_1 = \mathbf{\phi}_1^{(w)} \left( R_1, r_1 \right) + \mathbf{\phi}_1^{(w)} \left( R_2, r_2 \right) + \mathbf{\phi}_1^{(w)} \left( R_3, r_3 \right) . \]  

(2.13)

If we apply the Green's formula for six-dimensional integration to the first term of the right-hand side of Eq. (2.12), the surface term is dropped out, since \([\mathbf{\phi}_1 - \mathbf{\phi}_1^{(w)}]\) involves no plane wave, leading to

\[ \int \mathbf{\phi}_1(T + U_1 - E) \partial \mathbf{F} \, d\tau = -\frac{1}{3} \int (T + U_1 + U_2 + U_4 - E) \mathbf{\Pi}_1 \partial \mathbf{F} \, d\tau \]

\[ + \int \mathbf{\phi}_1^{(w)} (T + U_1 + U_2 + U_4 - E) \partial \mathbf{F} \, d\tau . \]  

(2.14)

Here we have used the relation \((T + U_1 - E) \mathbf{\phi}_1 = 0\). Remembering the relation

\[ (T + U_1 + U_2 + U_4 - E) \mathbf{\Pi}_1 = (T + U_1 + U_2 + U_4 - E) \partial \mathbf{\Pi} , \]  

(2.15)

the first term on the right-hand side of Eq. (2.14) is of second order in the error of the total wave function. Using also the adjoint relation of Eq. (2.15), we finally obtain the following variational expression for the scattering amplitude \( f(\theta) \):

\[ [f(\theta)] = f_1(\theta) - \frac{1}{3\pi} \int \mathbf{\phi}_1^{(w)} (T + U_1 + U_2 + U_4 - E) \mathbf{F} \, d\tau , \]  

(2.16)

which is accurate to second order in the error of the total wave function. It should be noted that Eq. (2.16) is valid above as well as below deuteron-breakup.

§ 3. Extended resonating-group method

In this section, we apply the variational principle to the calculation on the n-d s-state with any effective central potential of Serber-type.
3.1. Continuum states

For a Serber potential, the totally antisymmetric component \( \psi^a \) does not appear in the Schrödinger equation and we take

\[
\mathcal{H} = \psi'_1 \chi'' - \psi'' \chi' \quad \text{for Quartet} \tag{3.1}
\]

and

\[
\mathcal{H} = \frac{1}{2} \psi'_1 \chi' \chi'' - \frac{1}{2} \psi'' \chi' \chi''
- \frac{1}{2} (\psi' + \psi'') \chi'' + \frac{1}{2} (\psi' - \psi'') \chi' \chi'' \quad \text{for Doublet.} \tag{3.2}
\]

We assume

\[
\begin{align*}
\psi'_1 &= \frac{\sqrt{3}}{2} (\psi_1 - \psi_2), \tag{3.3a} \\
\psi'' &= -\psi_1 + \frac{1}{2} (\psi_1 + \psi_2), \tag{3.3b} \\
\psi' &= \psi_1 + \psi_2 + \psi_3, \tag{3.3c}
\end{align*}
\]

where the basis functions:

\[ \psi_i = \psi_i (R_i, r_i) \quad (i = 1, 2 \text{ and } 3) \tag{3.4} \]

are symmetric under the exchange between \( r_i \) and \( -r_i \), and have appropriate asymptotic forms. The adjoint functions \( \overline{\psi}'_i, \overline{\psi}''_i, \overline{\psi}'_i \) and \( \overline{\psi}_i \) are defined analogously.

Equation (2.16) then leads to

\[
[f(\theta)] = f_1(\theta) - \frac{1}{3\pi} \left[ \overline{\psi}_1 \left( (T - E) (\psi_1 - \psi_2) \right. + \left. \left( v_1 + \frac{1}{2} v_1 \right) \psi_1 - \left( v_1 + v_2 - \frac{1}{2} v_3 \right) \psi_2 \right] d\tau \quad \text{for Quartet} \tag{3.5}
\]

and

\[
[f(\theta)] = f_1(\theta) - \frac{1}{3\pi} \left[ \overline{\psi}_1 \left( (T - E) \left( \psi_1 + \frac{1}{2} \psi_2 \right) \right. \\
+ \left. \left( v_1 + \frac{1}{8} (v_1 + 9V_2) \right) \psi_1 + \left( \frac{1}{2} (v_1 + v_2) \right. \right. \\
+ \left. \left. + \frac{1}{8} (v_1 + 9V_3) \right) \psi_2 \right] d\tau \quad \text{for Doublet,} \tag{3.6}
\]

where \( v_i = V^+ (r_i) \quad (i = 1, 2 \text{ and } 3) \) is the potential in the triplet even state, and \( V_i = V^+ (r_i) \) that in the singlet even state.
After angular analysis, Eqs. (3.5) and (3.6) reduce to the usual variational principle for the $s$-phase shift:

$$
\left[ \frac{1}{k \cot \delta} \right] = \frac{1}{k \cot \delta_i} - \frac{1}{3 \pi} \int u_i L[u_i; E] d\tau \quad (3.7)
$$

with

$$
\int d\tau = \frac{8\pi^3}{3} \int_0^\infty dR_i \cdot R_i^2 \int_0^\infty dr_i \cdot r_i^2 \int_0^1 dx_i, \quad (i = 1, 2 \text{ or } 3) \quad (3.8)
$$

$x_i$ being the cosine of the angle between $\mathbf{R}_i$ and $\mathbf{r}_i$. Here we have defined

$$
L[u_i; E] = (T - E) (u_i - u_e) + \left( v_1 + \frac{1}{2} v_2 \right) u_1 - \left( v_1 + v_2 - \frac{1}{2} v_3 \right) u_2 \quad \text{for Quartet}, \quad (3.9)
$$

$$
L[u_i; E] = (T - E) \left( u_i + \frac{1}{2} u_e \right) + \left( v_1 + \frac{1}{8} (v_2 + 9V_3) \right) u_1 + \left( \frac{1}{2} (v_1 + v_2) + \frac{1}{8} (v_2 + 9V_3) \right) u_2 \quad \text{for Doublet}, \quad (3.10)
$$

where

$$
T = -\frac{1}{4} \sum_i \left( \frac{3}{4} \frac{\partial^2}{\partial R_i^2} + \frac{\partial^2}{\partial r_i^2} \right) R_i R_i
$$

$$
- \left( \frac{3}{4} \frac{\partial}{r_i} + \frac{1}{r_i^2} \right) \frac{\partial}{\partial x_i} (1 - x_i) \frac{\partial}{\partial x_i}, \quad (i = 1, 2 \text{ or } 3) \quad (3.11)
$$

$$
E = \frac{3}{4} \rho^2 + E_d, \quad (3.12)
$$

$E_d$ being the deuteron ground state energy, and

$$
u_i = u(R_i, r_i, x_i) \quad (i = 1, 2 \text{ and } 3) \quad (3.13)
$$

are the $s$-wave part of $\psi_i$, normalized such that

$$
u_i \xrightarrow{R_i \to \infty} \sin(kR_i + \delta_i) \phi(r_i) \quad (3.14)
$$

with

$$
4\pi \int_0^{\infty} \psi^2(r) r^2 dr = 1. \quad (3.15)
$$

* We use the units in which $\hbar = M = 1$, $M$ being the nucleon mass. In numerical evaluations, we take $\hbar \gamma M = 41.47 \text{ MeV} \cdot \text{fm}^3$. 
The trial phase shift $\delta_i$ is given by the relation

$$\int (u_i - u_j) \phi(r_i) d^3 r_i \xrightarrow{\text{var}} \sin \left( \frac{k R_i + \delta_i}{k R_i \cos \delta_i} \right)$$

(3.16)

for the quartet state and by a similar relation for the doublet state. When $k$ is zero, Eq. (3.7) represents the variational principle for the scattering length $a$:

$$[a] = a_i + \frac{1}{3\pi} \int u_i L[u_i; E_d] d\tau$$

(3.17)

with

$$u_i \xrightarrow{\text{var}} (1 - a_i/R_i) \phi(r_i).$$

(3.18)

The trial scattering length $a_i$ is given by the relation

$$\int (u_i - u_j) \phi(r_i) d^3 r_i \xrightarrow{\text{var}} 1 - a_i/R_i$$

(3.19)

for the quartet state and by a similar relation for the doublet state.

Equation (3.17) is an upper bound of $a$ for the quartet state.\(^{18}\) In the doublet state, there exists a bound state so that Eq. (3.17) should be modified to give an upper bound of $2a$ as follows:\(^{19}\)

$$[2a] = 2a + \frac{1}{3\pi} \int u_i L[u_i; E_d] d\tau$$

(3.20)

where $\omega_i$ is a trial function for the triton ground state satisfying

$$\int \omega_i L[\omega_i; E_d] d\tau < 0.$$

(3.21)

Now, in our variational calculation, we assume $u_i$ and $\omega_i$ to be of the form

$$u_i = [F(R_i)/R_i] \phi(r_i) f(r_i) f(r_k)$$

(3.22)

and

$$\omega_i = [F(R_i)/R_i] \phi(r_i) f(r_i) f(r_k);$$

(3.23)

with

$$f(r) \xrightarrow{\text{var}} 1,$$

(3.24)

where $i, j$ and $k$ are the permutations of 1, 2 and 3. Here we have introduced the pair correlation function $f(r)$ in order to take account of the distortion induced
A Variational Calculation on the n-d System

directly by the nuclear force. In the limiting case where the potential has an infinitely repulsive core, \( f(r) \) must vanish for any \( r \) less than the core radius. On the contrary, if we put everywhere \( f(r) = 1 \), we are led to the usual resonating-group model. Equation (3.22) implies that inelastically scattered waves are neglected.

According to Eqs. (3.14) and (3.18), \( F(R) \) satisfies the asymptotic condition:

\[
F(R) \xrightarrow{R \to \infty} \begin{cases} 
\frac{\sin (kR + \theta_i)}{k \cos \theta_i} & \text{for } k > 0, \\
R - a_1 & \text{for } k = 0,
\end{cases}
\]

while we put

\[
F(0) = F_B(0) = F_B(\infty) = 0.
\]

Substituting Eqs. (3.22) and (3.23) into Eqs. (2.7), (3.17) and (3.18), and performing integration over \( r_i \) and \( x_i \), we have

\[
\left[ \frac{1}{k \cot \theta_i} \right] = \frac{1}{k \cot \theta_i} - \int_0^\infty F(R) \mathcal{J}[F(R); k^2] dR,
\]

for Quartet

\[
\mathcal{J}^t[a] = \mathcal{J}^1[a] + \int_0^\infty F(R) \mathcal{J}[F(R); 0] dR
\]

and

\[
\mathcal{J}^d[a] = \mathcal{J}^1[a] + \int_0^\infty F(R) \mathcal{J}[F(R); 0] dR
\]

for Doublet,

where

\[
\mathcal{J}[F(R); k^2] = A(R) \frac{d^2 F(R)}{dR^2} + \frac{dA(R)}{dR} \frac{dF(R)}{dR} + k^2 A(R) F(R) - Q(R) F(R)
\]

\[
- \int_0^\infty B(R, S) F(S) dS - k^2 \int_0^\infty D(R, S) F(S) dS
\]

with \( A(R) \), \( Q(R) \), \( B(R, S) \) and \( D(R, S) \) given in the Appendix. Equations (3.28) \( \sim \) (3.30) are the variational formulae for the equivalent two-body problem described by the equation of motion

\[
\mathcal{J}[F(R); k^2] = 0.
\]

Therefore, once an explicit form of \( f(r) \) is given, Eq. (3.32) determines the
best form of \( F(R) \), giving the most accurate values of \( \delta \), and \( a_i \). With this \( F(R) \), Eqs. (3·28) ~ (3·30) reduce simply to

\[
[1/k \cot \delta] = 1/k \cot \delta, \tag{3·33}
\]

and

\[
[a] = a_i \tag{3·34}
\]

for both the quartet and doublet states. Equation (3·34) is an upper bound of \( a \) for the doublet state as well, if we guarantee

\[
\int_0^\infty F_\theta(R) \left[ F_\theta(R); 0 \right] dR < 0, \tag{3·35}
\]

which is fulfilled in practice, as will be shown later.

If we further put

\[
G(R) = \sqrt{A(R)} F(R), \tag{3·36}
\]

Eq. (3·32) becomes

\[
\frac{d^2 G(R)}{dR^2} + k^2 G(R) = U(R) G(R)
\]

\[+ \int_0^\infty K(R, S) G(S) dS + k^2 \int_0^\infty N(R, S) G(S) dS, \tag{3·37}
\]

where

\[
U(R) = \left[ A(R) Q(R) + \left\{ 2A(R) \frac{d^2 A(R)}{dR^2} - \left( \frac{d A(R)}{dR} \right)^2 \right\} \right] / A(R), \tag{3·38}
\]

\[
K(R, S) = -\frac{1}{\sqrt{A(R)}} B(R, S) \frac{1}{\sqrt{A(S)}}, \tag{3·39}
\]

and

\[
N(R, S) = -\frac{1}{\sqrt{A(R)}} D(R, S) \frac{1}{\sqrt{A(S)}}, \tag{3·40}
\]

Equation (3·37) is of the same form as the usual resonating-group model and we may call it an extended resonating-group model improved so as to take in the pair correlation functions. Relating to \( G(R) \), there is the following important physical meaning. The trial function (3·22) is put into

\[
u_i = [G(R_i) / R_i] \phi_i(r_i; R_i, x_i), \tag{3·41}
\]

where we have defined

\[
\phi_i(r_i; R_i, x_i) = \psi(r_i) f(r_i) f(r_k) / \sqrt{A(R_i)}. \tag{3·42}
\]

By virtue of (A·1), we have
so that \( \phi_d \) is interpreted as the deuteron wave function distorted by the \( n-d \) interaction. Equation (3.41) then shows that \( G(R) \) represents the \( n-d \) relative motion in our extended resonating-group model.

### 3.2. Bound state

The variational principle for the bound state is given by

\[
\int \nabla' H \nabla d\tau \geq E_r,
\]

where \( E_r \) is the exact ground state energy of triton, \( \nabla' \) the trial function of the form (3.2) and \( H \) the total Hamiltonian. As in the preceding subsection, the left-hand side of the inequality (3.44) is expressed in terms of \( u_t \).

Now, we assume \( u_t \) to be of the same form as Eq. (3.22) with the boundary condition

\[
F(0) = F(\infty) = 0.
\]

The inequality (3.44) then leads to

\[
\frac{3}{4} \int_0^\infty F(R) \left\{ -\frac{dA(R)}{dR} \frac{d^2 F(R)}{dR^2} - \frac{dA(R)}{dR} \frac{dF(R)}{dR} + Q(R) F(R) \right\} dR + \int_0^\infty F(R) \left\{ A(R) F(R) \right\} dR + E_d \\
\geq E_r.
\]

The left-hand side of the inequality (3.46) has its minimum when \( F(R) \) is the ground-state eigenfunction of the equation

\[
\alpha [F(R); -\kappa^2] = 0.
\]

The lowest upper bound for the triton energy \( E_n \) is therefore given by

\[
E_n = E_d - \frac{3}{4} \kappa^2,
\]

where \( -\kappa^2 \) is the lowest eigenvalue of Eq. (3.47). It should be remembered that the inequality (3.21) is always guaranteed unless \( \kappa = 0 \), if we identify the solution of Eq. (3.47) with \( F_n(R) \); indeed, Eq. (3.47) is converted into

\[
\int \nabla' (H - E_d) \nabla d\tau = (E_n - E_d) \int \nabla' \nabla d\tau,
\]
where the left-hand side is equal to

$$3 \int_{\Re}^{\infty} F(R) \mathcal{J} [F(R); 0] dR,$$

(3.50)

while the right-hand side is negative unless $\kappa = 0$.

§ 4. Numerical example

We assume a two-nucleon potential of Gaussian form:

$$\mathcal{V}(r) = V_0 \exp \left[ - \frac{r^2}{\alpha^2} \right].$$

(4.1)

The values of the potential parameters are given in Table I, where the low-energy two-nucleon data to which the parameters are fitted are also shown. The exact deuteron wave function is evaluated numerically to construct the trial function. The correlation function is also assumed to be of Gaussian form:

$$f(r) = 1 - \alpha \exp \left( -\beta r^2 \right), \quad (\beta > 0)$$

(4.2)

where $\alpha$ and $\beta$ are variational parameters.

In our variational procedure, we solve Eqs. (3.32) or (3.37) and (3.47) for each value of $\alpha$ and $\beta$, and search for the minima of $a_i$ and $-\kappa^2$ and the stationary values of $1/k \cot \delta_i$.

Table I. The two-nucleon potential parameters and low-energy two-nucleon data. $a$ is the scattering length and $r_e$ the effective range.

<table>
<thead>
<tr>
<th></th>
<th>$V_0$ (MeV)</th>
<th>$\alpha$ (fm)</th>
<th>$\beta$ (fm)</th>
<th>$r_e$ (fm)</th>
<th>$E_a$ (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>triplet</td>
<td>-67.0</td>
<td>5.423</td>
<td>1.765</td>
<td>-2.224</td>
<td></td>
</tr>
<tr>
<td>singlet</td>
<td>-31.1</td>
<td>1.815</td>
<td>-23.71</td>
<td>2.740</td>
<td></td>
</tr>
</tbody>
</table>

4.1. Continuum states

Equation (3.32) or Eq. (3.37) is put into a system of finite-difference equations and solved numerically for incident energies below 15 MeV.

In the quartet state, $1/k \cot \delta_i$ depends little on $\alpha$ and $\beta$, but has broad maxima at various values of them, depending on the incident energy. The values of $\alpha$ and $\beta$ giving these maxima lie in the region: $-0.5 \leq \alpha \leq 1, 0.2 \leq \beta \leq 0.3$ (in fm$^{-2}$). In the doublet state, $1/k \cot \delta_i$ has maxima at $\alpha = -2, \beta = 0.2$ fm$^{-1}$, almost independently of the incident energy. Figure 2 shows the values of $k \cot \delta_i$ corresponding to the maxima of $1/k \cot \delta_i$ at each incident energy. For zero incident energy, the variation of $-1/k \cot \delta_i$, that is, $a_i$, with $\alpha$ and $\beta$ is illustrated in Fig. 3. The behavior of the $n-d$ relative wave function $G(R)$ is shown in Fig. 4.

Now, our trial function (3.22) is particularly useful as an approximate wave function to elucidate the interaction mechanisms of $n-d$ scattering. Substituting
Fig. 2. The calculated values of $k \cot \delta_i$ (solid curves). The circles are experimental points. The result of the usual resonating-group model is also shown (dashed curves). For the doublet state, the effective range formula (5·3) gives a curve which is graphically the same as the solid curve. The dot-dashed curve represents the result of Eq. (4·4).

Fig. 3. The variation of $-1/k \cot \delta_i$ for $E_L=0$, namely, the scattering length $a_i$, with $\alpha$ and $\beta$.

Fig. 4. The zero-energy $n-d$ relative wave function $G(R)$ (solid curves) and the asymptote of $G(R)$ (dot-dashed lines). The result of the usual resonating-group model (RGM) is also shown (dashed curves).
\( \mathcal{T}_s \) as defined by Eqs. (3·1) and (3·2) for \( \mathcal{T}_s \), in Eqs. (2·5) and (2·7), we obtain the integral formulae for the \( s \)-wave phase shift:
\[
\frac{1}{k \cot \delta_0} = - \frac{1}{3 \sqrt{\pi} k} \int \sin \frac{kR_1}{R_1} \phi(r_1) \times \left[ \frac{1}{2} v_2 \psi_1 - \frac{1}{2} v_1 \psi_2 \right] d\tau
\]
for Quartet (4·3)

and
\[
\frac{1}{k \cot \delta_0} = - \frac{1}{6 \sqrt{\pi} k} \int \sin \frac{kR_1}{R_1} \phi(r_1) \times \left[ \frac{1}{4} (v_1 + 9V_1) \psi_1 + \frac{1}{4} (v_2 + 9V_2) \psi_2 \right] d\tau
\]
for Doublet. (4·4)

Each term in the square brackets of Eqs. (4·3) and (4·4) corresponds to a definite interaction mechanism; the first term to the direct process, the second to the knockon and the last to the pickup. Figure 5 shows the energy dependence of these processes in the doublet state.

![Fig. 5. The effective range formula (5·4) and its extrapolation to negative energies (solid curves). Each term of Eq. (5·4), ERF1 and ERF2, and the contribution of each term of Eq. (4·4), related to the corresponding scattering process, are also shown. Circles are experimental points.]

4.2. **Bound state**

We solve Eq. (3·47) under the condition (3·45). Figure 6 shows the varia-
tion of the eigenvalue $-\epsilon^2$ with $\alpha$ and $\beta$. The lowest value for the triton ground-state energy is found to be $-9.53$ MeV when $\alpha = -6$ and $\beta = 0.1$ fm$^{-1}$. Figure 7 shows the behavior of the inter-cluster wave function $G_\beta(R)$ defined in the same way as Eq. (3.36) by

$$G_\beta(R) = \sqrt{A(R) F(R)}, \quad (4.5)$$

which represents the motion of a neutron relative to a deuteron-cluster in the triton, and is normalized such that

$$4\pi \int_0^\infty G_\beta^2(R) dR = 1. \quad (4.6)$$

In Table II, we summarize our results in comparison with low-energy $n-d$ data.
Table II. The low-energy \( n-d \) quantities. RGM is the result of the usual resonating-group method. Experimental values are from Ref. 22).

<table>
<thead>
<tr>
<th></th>
<th>( \langle \ell_a \rangle ) (fm)</th>
<th>( \langle \ell_d \rangle ) (fm)</th>
<th>( E_r ) (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RGM</td>
<td>6.33</td>
<td>2.10</td>
<td>-7.36</td>
</tr>
<tr>
<td>The present work</td>
<td>6.32</td>
<td>0.77</td>
<td>-9.53</td>
</tr>
<tr>
<td>Experiment</td>
<td>6.35 ± 0.02</td>
<td>0.65 ± 0.04</td>
<td>-8.48</td>
</tr>
</tbody>
</table>

§ 5. Discussion

Our variational calculations are on the whole in good agreement with experiment, considering that we have assumed an effective central local potential without repulsive core and neglected inelastically scattered waves. The usual resonating-group model has been considerably improved in the doublet state, reflecting the fact that the distortion of the wave function induced directly by the nucleon-nucleon interaction is large. This will be visualized more clearly in terms of the angle-averaged deuteron wave function \( \bar{\phi}_d \) defined by

\[
\bar{\phi}_d(r; R) = \sqrt{\frac{1}{\pi}} \int_0^\infty \, \phi_d^2(r_1; R_1, x_1) \, dz_1/2
\]

and the r.m.s. radius of deuteron \( \bar{r}_d \) defined by

\[
\bar{r}_d = \sqrt{\frac{2}{\pi}} \int_0^\infty \, dr_1 \, \int_0^\infty \, dx_1 \, r_1^2 \, \phi_d^2(r_1; R_1, x_1).
\]

Figure 8 shows the behavior of \( \bar{\phi}_d \) and \( \bar{r}_d \) for the doublet state; the target deuteron is at first enlarged slightly and then strongly compressed as the incident

![Fig. 8. The angle-averaged deuteron wave function \( \bar{\phi}_d(r, R) \) and the r.m.s. radius of deuteron \( \bar{r}_d \) for various \( n-d \) distances.](https://academic.oup.com/ptp/article-abstract/64/1/162/1904686)
neutron approaches closer. The behavior of $k \cot \theta$ is excellently reproduced near zero energy as well as above deuteron-breakup. By contrast, in the quartet state, the distortion of the wave function has proved again negligibly small, justifying the usual resonating-group model.

The calculated binding energy of triton, on the other hand, exceeds the observed one, as it should be from our use of the simple central potential. We should therefore not insist too much on reproducing accurately the experimental values with simple potentials. Instead, we intend here to show the usefulness of the variational principle with such a simple trial function as we have used, and to elucidate microscopically the interaction mechanisms of the $n$-$d$ system.

Now, for the doublet state, the well-known effective range formula

$$k \cot \theta = -A + Bk^2 - \frac{C}{1 + Dk^2}$$

(5·3)

is proposed empirically. Our calculation also can be fitted by this formula quite well as depicted in Fig. 2 with $A = 0.3255 \, \text{fm}^{-1}$, $B = 0.7582 \, \text{fm}$, $C = 0.9742 \, \text{fm}^{-1}$ and $D = 187.1 \, \text{fm}^2$. The formula (5·3) is put into a combination of the usual effective range expansions of $k \cot \theta$ as follows:

$$1/k \cot \theta = \text{ERF}_1 + \text{ERF}_2 ,$$

(5·4)

where

$$1/\text{ERF}_1 = -1/a_s + \frac{1}{2} r_{uL} k^2$$

(5·5)

and

$$1/\text{ERF}_2 = -1/a_L + \frac{1}{2} r_{uL} k^2$$

(5·6)

with $a_s = 2.867$, $r_{uL} = 1.589$, $a_L = -2.098$ and $r_{uL} = 46.27$ (in fm). In Fig. 5, we show each contribution of ERF1 and ERF2 and compare them with the contributions of the various processes. This comparison reveals that ERF1 is attributed mainly to the direct- and knockon processes, while ERF2 mainly to the pickup process. At the same time, Fig. 5 shows that the direct- and knockon processes contribute in a similar manner.

Figure 5 also shows the extrapolation of the formula (5·4) to the negative energy; the intersection with the curve $-1/\sqrt{-k^2}$ determines the triton energy. It turns out from Fig. 5 that the doublet state is dominated mainly by ERF1 except near zero energy, but there is a crucial interference between ERF1 and ERF2 in determining the doublet scattering length and the triton energy. In other words, the doublet scattering length is determined by an almost complete cancellation between the short-range direct- and knockon processes and the long-range pickup process. This is seen also from Fig. 9 which shows the dependence of the left-
hand sides of Eqs. (4·3) and (4·4) at zero energy on the value of \( R_\text{max} \), say \( R_\text{max} \), at which the integration is cut off. In contrast to the doublet state, the quartet state is dominated almost exclusively by the pickup process, as Fig. 9 shows.

Now, Petrov\(^5\) has made a calculation on the \( n-d \) system with a Gaussian potential by a separable expansion method of the two-body \( t \)-matrix based on the Faddeev equations. We have also made our variational calculation with his potential, obtaining \( \tilde{a} = 6.27 \) (6.29) fm, \( \tilde{a} = 0.67 (-0.42) \) fm and \( E_R = -9.78 (-9.95) \) MeV, where the values in the parentheses are Petrov’s results. Except for the doublet scattering length \( \tilde{a} \), our results agree well with Petrov’s. We only remark here that the value of \( \tilde{a} \) is changeable, as Figs. 4 and 5 indicate, depending on the computational accuracy; indeed, Fig. 4 shows that the zero-energy wave function \( G(R) \) has non-vanishing curvature even beyond 30 fm due to the long-range part of the kernel in Eq. (3·37), requiring accurate evaluation over wide range.

The accuracy of our calculation may be measured by comparing our variationally determined values of \( k \cot \delta \), with those evaluated by Eqs. (4·3) and (4·4), since the former are accurate to second order in the error of the wave function while the latter are accurate only to first order. Figure 2 shows this comparison, the former giving \( \tilde{a} \) of 0.77 fm while the latter that of 0.45 fm. Note that both coincide if we assume the usual resonating-group model, as is the case of the quartet state.

Finally, we discuss our results in the light of the Faddeev equations. If our trial functions (3·1) and (3·2) are supposed to be the true solutions to the Schrödinger equation (2·5), then the Faddeev equations (2·4) should lead to

\[
(T + v_t - E) \psi_t = \frac{1}{2} v_t (\phi_j + \phi_k) \quad \text{for Quartet}
\]

and

\[
(T + v_t - E) \psi_t = - \frac{1}{4} (v_t - V_c) (\phi_j + \phi_k)
\]
A Variational Calculation on the n-d System

\[ -\frac{1}{2} \left[ (V_1 + V_2) \psi_1 + V_3 \psi_3 + V_4 \psi_4 \right] \quad \text{for Doublet}, \]

\[ (5\cdot8) \]

\( i, j \) and \( k \) being the permutations of 1, 2 and 3. Equations (5·7) and (5·8) reduce to single equations with \( i=1, j=2 \) and \( k=3 \).

To see how well our trial functions satisfy Eqs. (5·7) and (5·8), we multiply these equations by \( \phi_i(r_i) \) and integrate them over \( r_i \), obtaining

\[ (5\cdot9) \]

\[ (5\cdot10) \]

where we have put

\[ (5\cdot11) \]

Equations (5·9) and (5·10) are the projection of the Faddeev equations (5·7) and (5·8) onto the deuteron ground state. We now substitute our trial functions (3·4) on the right-hand sides of Eqs. (5·9) and (5·10), and solve them for \( \psi_F \) under appropriate boundary conditions. If the trial functions are the exact solutions to Eqs. (5·7) and (5·8), the equality (5·11) should hold rigorously. In Figs. 7 and 10, we compare the solution \( \psi_F \) to Eq. (5·9) and (5·10) with the right-hand side of Eq. (5·11) for the s-state. In the doublet state, there is a fairly good agreement between them for both the scattering states and the bound one.

In the quartet state, however, the agreement is poor, in spite of our success in reproducing the quartet phase shift. In other words, the resonating-group model seems quite adequate for the quartet state, but the wave function in this model is not a good solution to the Faddeev equation (5·7). This is because the quartet phase shift is given by the integral formula (4·3) which does not change by replacing \( \psi_i \) with \( \psi_i - \omega^* \), where \( \omega^* \) is an arbitrary function of full symmetry under nucleon exchange. Therefore, such a symmetric component of the Faddeev solution, if any, makes no contribution to the phase shift, but may bring some difference between the Faddeev solution and the resonating-group wave function. In the doublet state, on the contrary, any symmetric component of the Faddeev solution contributes to the phase shift and has a physical meaning.
Fig. 10. The comparison between the n-d relative wave function $G(R)$ (solid curves) and the s-state solution to the projected Faddeev equations (5.9) and (5.10) (dashed curves).

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Appendix

\[ A(R_3) = 2\pi \int_0^\infty dr_1 \cdot r_1 \phi^*(r_1) \int_{-1}^1 [f(r_2) f(r_3)]^* dx_1, \quad (A \cdot 1) \]

\[ Q(R_3) = UD(R_0) + A'(R_1)/R_3 - \frac{8\pi}{3} \int_0^\infty dr_1 \cdot r_1 \phi^*(r_1) \]

\[ \times \int_{-1}^1 f(r_2) f(r_3) \left[ \phi(r_1) \left( \frac{3}{4} d_{R_1} + d_{r_1} \right) f(r_2) f(r_3) \right. \]

\[ + 2V_r \phi(r_1) \cdot \nabla_r f(r_2) f(r_3) \left. \right] dx_1, \quad (A \cdot 2) \]

\[ UD(R_3) = \frac{\pi}{3} \int_0^\infty dr_1 \cdot r_1 \phi^*(r_1) \int_{-1}^1 dx_1 [f(r_2) f(r_3)]^2 \]

\[ \times \left[ \begin{array}{l}
4 \nu(r_2) \\
\nu(r_2) + 9V(r_1)
\end{array} \right] \quad \text{for Quartet}, \quad (A \cdot 3) \]

\[ B(R_1, R_3) = \nu B_{\text{inst}}(R_1, R_3) + B_{\text{knock}}(R_1, R_3) + \nu B^{(\text{Q})}_{\text{pick}}(R_1, R_3) - 5\nu B^{(\text{D})}_{\text{pick}}(R_1, R_3), \quad (A \cdot 4) \]

where

\[ \nu = \begin{cases} 1 & \text{for Quartet}, \\ -\frac{1}{2} & \text{for Doublet}, \end{cases} \quad (A \cdot 5) \]

\[ B_{\text{inst}}(R_1, R_3) = \frac{8\pi}{3} \left( \frac{4}{3} \right)^2 R_1 R_3 \int_{-1}^1 dx_1 (D_1 + D_2 - D_3), \quad (A \cdot 6) \]

\[ D_1 = \phi(r_1) f(r_2) f(r_3) \left[ \phi(r_1) d_{R_1} f(r_2) f(r_3) \right. \]

\[ + 2V_r \phi(r_1) \cdot \nabla_r f(r_2) f(r_3) \left. \right] + (R_1 \leftrightarrow R_2), \quad (A \cdot 7) \]

\[ D_2 = \phi(r_1) \phi(r_2) \nabla_{R_1} \left[ f(r_2) f(r_3) \right] \cdot \nabla_{R_1} \left[ f(r_1) f(r_3) \right], \quad (A \cdot 8) \]

\[ D_3 = \phi(r_1) f(r_2) f(r_3) \nabla_{R_1} \left[ f(r_2) f(r_3) \right] \cdot \nabla_{R_1} \phi(r_2) + (R_1 \leftrightarrow R_2), \quad (A \cdot 9) \]

where \((R_1 \leftrightarrow R_2)\) means the same terms as the preceding ones except for \(R_1\) and \(R_2\) interchanged.

\[ B_{\text{knock}}(R_1, R_2) = \frac{4\pi}{9} \left( \frac{3}{4} \right)^2 R_1 R_2 \int_{-1}^1 dx \phi(r_2) \phi(r_2) f(r_1) f(r_2) f^*(r_3) \]
\begin{equation}
B_{\text{pick}}^{(Q)}(R_1, R_2) = \frac{2\pi}{3} (\frac{4}{3})^4 R_1 R_2 \int_0^1 dx \left[ \phi(r_1) \{v(r_1) + v(r_2)\} \phi(r_2) + 4\phi'(r_1) \frac{r_1 \cdot r_2 \phi'(r_2)}{r_1 \cdot r_2} f(r_1) f(r_2) f'(r_2) \right],
\end{equation}

\begin{equation}
B_{\text{pick}}^{(D)}(R_1, R_2) = \frac{2\pi}{3} (\frac{4}{3})^4 E_e R_1 R_2 \int_0^1 dx \phi(r_1) \phi(r_2) f(r_1) f(r_2) f'(r_2),
\end{equation}

\begin{equation}
D(R_1, R_2) = \frac{9}{4E_e} B_{\text{pick}}^{(D)}(R_1, R_2).
\end{equation}

**References**

7) 4\pi^2(r_1) \int_0^1 dx x \phi'(r_1) \phi'(r_2) f(r_1) f(r_2) f'(r_2),
A Variational Calculation on the n-d System

T. Ohmura, Prog. Theor. Phys. 22 (1959), 34.
14 L. D. Faddeev, ZhETF 39 (1960), 1459; (JETP-Soviet Phys. 12 (1961), 1014.)