AN UPPER BOUND ON THE NEUTRON-DEUTERON ^2S SCATTERING LENGTH*

L. M. Delves, J. N. Lyness, and J. M. Blatt
University of New South Wales, Sydney, Australia and New York University, New York, New York
(Received 13 April 1964)

The zero-energy experiments on n-d scattering[1] lead to a set of quadratic equations for the two scattering lengths a_2 (doublet state) and a_4 (quartet state). This set of equations has two solutions, namely,

Solution 1: $a_2 = (0.7 \pm 0.3) \times 10^{-13}$ cm,

$a_4 = (6.4 \pm 0.1) \times 10^{-13}$ cm;

Solution 2: $a_2 = (8.3 \pm 0.1) \times 10^{-13}$ cm,

$a_4 = (2.6 \pm 0.2) \times 10^{-13}$ cm.

No decision between these solutions is possible on the basis of the data on n-d scattering.

For this reason, as well as others, it is of interest to make a theoretical calculation with the best available nuclear two-body force laws. This Letter reports the results obtained to date.

Spruch and Rosenberg[2] have developed a method of finding an upper bound to the scattering length a_2; since the state concerned is the same state which gives rise to the ground state of the triton, the earlier analysis of triton states with $J = \frac{1}{2}$ and even parity[3] can be used for this calculation.

The simplest type of scattering function, obtained in the absence of spin-orbit coupling and repulsive cores, has the form

$$[f_{\alpha\alpha}(\rho_3)/\rho_3][u(z)/z]\tfrac{1}{2}(Y_1 - Y_{3,2}), \qquad (1)$$

where $z = r_{12}$ is the distance between particles 1 and 2 (which make up a deuteron), $u(z)$ is the usual radial wave function of that deuteron, ρ_3 is the distance between the center of gravity of particles 1 and 2, and particle number 3; $f_{\alpha\alpha}(\rho_3)$ is the radial wave function for the scattering, going asymptotically like

$$f_{\alpha\alpha}(\rho_3) \cong \rho_3 - a_t, \qquad (2)$$

where a_t is the neutron-deuteron scattering length; and Y_1 and $Y_{3,2}$ are two of the Euler-angle-spin-isospin functions of reference 3. The function (1) is antisymmetric under exchange of particles 1 and 2, but not under permutations involving particle 3.

The actual function used in our calculation is a generalization of (1), necessitated by the following aspects of the realistic problem:

(A) Hard cores.—The wave function must vanish when either r_{13} or r_{23}, or both, are equal to the hard-core radius r_0. We introduce a function $g_{\alpha\alpha}(x)$ which has the properties

$$g_{\alpha\alpha}(r_0) = 0, \quad \lim_{x\to\infty} g_{\alpha\alpha}(x) = 1, \qquad (3)$$

and multiply (1) by the factor $g_{\alpha\alpha}(r_{13})g_{\alpha\alpha}(r_{23})$. Apart from the properties (3), the function g is undetermined and its detailed behavior is adjustable for the purposes of a variational calculation.

(B) Exchange symmetry.—In the isotopic spin formalism (which we use) the total wave function must be antisymmetric under exchange of any two particles. Let $\psi_S(1,2,3)$ be the function used so far, i.e., the function describing a deuteron consisting of particles 1 and 2, and a scattered neutron labeled particle number 3; then a properly antisymmetrized scattering function has the form

$$\psi_a = 3^{-1/2}[\psi_S(1,2,3) + \psi_S(2,3,1) + \psi_S(3,1,2)]. \qquad (4)$$

(C) Spin-orbit forces, including the tensor force.—When spin-orbit and tensor forces are included, the deuteron wave function has both $L = 0$ and $L = 2$ components, with radial wave functions conventionally called $u(z)$ and $w(z)$. The function (1) is then replaced by the more complex form

$$f_{\alpha\alpha}(\rho_3)\Phi_\alpha, \qquad (5)$$

where Φ_α is a "surface function" defined explicitly by Eq. (5.3) of Delves and Derrick.[4]

Furthermore, the spin-orbit coupling implies that a pure S wave is not a solution of the scattering problem. The function (5) is the "α wave," one of the two eigenstates of the scattering matrix. The other eigenwave, the "β wave," also contributes in general. Its surface function Φ_β is defined explicitly in Eq. (5.3) of reference 4, also. The unsymmetrized scattering function $\psi_S(1,2,3)$ is then given by

$$\psi_S(1,2,3) = g_{\alpha\alpha}(r_{13})g_{\alpha\alpha}(r_{23})f_{\alpha\alpha}(\rho_3)\Phi_\alpha + \epsilon_T g_{\alpha\beta}(r_{13})g_{\alpha\beta}(r_{23})f_{\alpha\beta}(\rho_3)\Phi_\beta, \qquad (6)$$

where $g_{\alpha\alpha}$ and $f_{\alpha\alpha}$ satisfy conditions (3) and (2),

respectively, $g_{\alpha\beta}$ also satisfies conditions (3), and $f_{\alpha\beta}$ has the asymptotic form

$$f_{\alpha\beta}(\rho_3) \cong 3/\rho_3{}^3. \tag{7}$$

ϵ_T is a variational parameter; it has the interpretation of a trial mixing parameter.

(D) Requirement of an upper bound.—The antisymmetric function (4) formed from (6) is a permissible trial function in a variation principle for the scattering length, enabling us to use an approximate trial value a_t in the asymptotic form (2), and deduce an improved value whose error is of the order of the square of the error of the trial value. However, this trial function is not good enough to determine the sign of the remaining error. For this latter purpose, it is necessary[2] to add a multiple of a "successful" bound-state trial function $\Phi_B(1,2,3)$, where "successful" means that the expectation value of the Hamiltonian over Φ_B, called E_{Bt} henceforth, at least gives binding of the third particle, i.e., satisfies the condition

$$E_{Bt} < E_D = -2.226 \text{ MeV}. \tag{8}$$

Successful bound-state trial functions, in this sense, have been determined previously[5] for all presently popular two-body force laws, and these functions were used in the present calculation.

The full trial wave function adopted by us for n-d scattering then has the form

$$\psi_t = \psi_a + C\Phi_B, \tag{9}$$

where ψ_a is defined by (4) and (6), and C is a constant which must be adjusted afterwards to a specific value so as to obtain an upper bound on the computed scattering length.

Although it is the simplest possible function which can be used, (9) is of sufficient complexity to lead to fairly elaborate expressions for the relevant matrix elements of the Hamiltonian. All the expressions have been given previously by Delves and Lyness.[6] The formulas of reference 6 have been incorporated into a FORTRAN II code called SCANDAL; an improved version of this code, FAR-REACHING SCANDAL, uses alternative but equivalent formulas and allows the integrations to proceed farther out into the channel region.

We found that we had to integrate very far out indeed before the integrals converged. Channel radii of the order of 30 F proved just barely sufficient, while for checking purposes we have integrated out to 38 F. There are two reasons for this: (1) The exchange terms arising from the identity of the particles produce terms of type $u(r_{12})u(r_{23})$, where u is the radial deuteron wave function. Since the deuteron is only loosely bound, distances of order $r_{12} = 10$ F still contribute marginally, and the exchange terms therefore still contribute marginally at distance of order $r_{13} = 20$ F. (2) The wave functions $f_{\alpha\alpha}(\rho_3)\Phi$ and $f_{\alpha\beta}(\rho_3)\Phi_\beta$ have the property (as they must for the integrals to converge) that in the channel regions

$$(H - E_D) f_{\alpha\alpha}(\rho_3)\Phi_\alpha \to 0,$$
$$(H - E_D) f_{\alpha\beta}(\rho_3)\Phi_\beta \to 0. \tag{10}$$

However, the D-wave parts of the expressions for Φ_α and Φ_β contained in reference 4 represent only the leading terms in an exact solution of the wave equation in this region, and (10) is approached only rather slowly. This second cause of slow convergence can be eliminated by using more accurate forms for Φ_α and Φ_β, and we intend to do so in future calculations; however, the first cause is inherent in the physics of the problem.

We have investigated the three most realistic two-body potentials (Brueckner-Gammel,[7] Hamada-Johnston,[8] and Yale[9] potentials), with the following results:

Brueckner-Gammel: $a_2 < 3.0 \times 10^{-13}$ cm,

Hamada-Johnston: $a_2 < 4.9 \times 10^{-13}$ cm,

Yale: $a_2 < 5.2 \times 10^{-13}$ cm.

In every case, the upper bound on the doublet n-d scattering length a_2 is consistent with solution 1, and inconsistent with solution 2. In view of the rather crude trial function used, and the limited amount of variation of parameters carried out by us, the difference between the experimental solution 1 ($a_2 = 0.7 \times 10^{-13}$ cm) and our present upper bounds on a_2 cannot be considered as significant. The close correspondence between the results for the Hamada-Johnston and Yale potentials is to be expected, in view of the general similarity of these two potentials.

We are grateful to the Courant Institute, New York University, for the very generous amounts of IBM-7094 time made available for this investigation, and to the staff of the Institute for much appreciated help and advice.

*This work was supported in part by the U. S. Atomic Energy Commission Computing and Applied Mathematics Center, Courant Institute of Mathematical Sciences, New York University, under contract with the U. S. Atomic Energy Commission, and in part by the U. S. Air Force through Grant No. 62-400 to the University of New South Wales, Sydney, Australia.

[1]D. G. Hurst and J. Alcock, Can. J. Phys. 29, 36 (1951); E. O. Wollan, C. G. Shull, and W. C. Koehler, Phys. Rev. 83, 700 (1951).

[2]L. Spruch and L. Rosenberg, Phys. Rev. 116, 1034 (1959); L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. 118, 184 (1960); L. Rosenberg and L. Spruch, Phys. Rev. 121, 1720 (1961); Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. 130, 381 (1963).

[3]G. H. Derrick, Nucl. Phys. 16, 405 (1960); 18, 303 (1960).

[4]L. M. Delves and G. H. Derrick, Ann. Phys. (N.Y.) 23, 133 (1963).

[5]J. M. Blatt, G. H. Derrick, and J. N. Lyness, Phys. Rev. Letters 8, 323 (1962).

[6]L. M. Delves and J. N. Lyness, Nucl. Phys. 45, 296 (1963).

[7]K. A. Brueckner and J. L. Gammel, Phys. Rev. 109, 1023 (1958).

[8]T. Hamada and I. D. Johnston, Nucl. Phys. 34, 382 (1962).

[9]K. E. Lassila, M. H. Hull, H. M. Ruppel, F. A. McDonald, and G. Breit, Phys. Rev. 126, 881 (1962).

FURTHER RESULTS ON THE BINDING ENERGY OF THE TRITON*

J. M. Blatt and L. M. Delves
Courant Institute, New York University, New York, New York
and University of New South Wales, Sydney, Australia
(Received 13 April 1964)

In the course of an investigation of the neutron-deuteron scattering length[1] we noticed that a fairly simple modification of the code could be used to reinvestigate the binding energy of the triton with an improved trial function. The trial function (I, 9)[2] becomes a suitable trial function for a bound state merely by altering the asymptotic behavior (I, 2) and (I, 7) of the functions $f_{\alpha\alpha}(\rho)$ and $f_{\alpha\beta}(\rho)$; if both these functions decrease for large ρ sufficiently rapidly (e.g., exponentially), we satisfy all necessary conditions.

Furthermore, since the trial function used previously,[3] Φ_B, is contained in (I, 9), the new result must be an improvement on the old one. It is clearly of interest to ascertain the order of magnitude of this improvement.

An additional reason for further investigation arises from the work of Schiff[4] on the analysis of the scattering of fast electrons on tritons. Schiff suggests that the percentage of state No. 3, the S state of permutation symmetry $(2+1)$, may be larger than the $\frac{1}{4}\%$ or less found for the best available potentials[5-7] in reference 2. Schiff would like 4% or more for the probability of state No. 3. Referring to Formula (I, 1), we note that the amplitudes of state Nos. 1 and 3 are equal to each other in the main component of the "scattering-type" function ψ_a of (I, 9). Admixture of such a function would therefore tend to increase the percentage of state No. 3 in the over-all trial wave function.

In Tables I, II, and III, we present results for three new trial wave functions, namely: (A) wave function (I, 9) with $f_{\alpha\alpha}(\rho)$ and $f_{\alpha\beta}(\rho)$ decreasing exponentially for large ρ; (B) same as (A), except that ψ_a of (I, 9) has been separated into S-state (state Nos. 1, 2, 3), P-state (state Nos. 4, 5, 6, 7), and D-state (state Nos. 8, 9, 10) components, each with an adjustable linear coefficient; and (C) same as (B), except that the linear coefficients which appear in the previous calculation[3] in Φ_B, for state Nos. 1, 2, 3, 4, 6, 7, and a single coefficient for all the D states together, have been revaried.

The improvements obtained in the upper bound of the triton ground-state energy are very significant, and comparison of the old results (also given in the tables) with results for wave functions (A) and (C) indicates that there is no reason to believe that convergence has set in. Comparison of the results for wave functions (B) and (C) shows, however, that revarying the linear coefficients in the old wave function does not make any real difference.

The binding energy obtained from the "scattering-type" wave function or its modification according to scheme (B) is not better than the previously obtained binding energy, for any of these potentials. The large improvement results entirely from interference between the function Φ_a and the "old" function Φ_B.

The large improvement obtained by allowing some of the linear coefficients in ψ_a to vary independently [i.e., going from (A) to (B) in the