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Binding Energy of the Triton with the Hamada-Johnston Potential*

Chi-yu Hu
Department of Physics and Astronomy, California State College, Long Beach, California 90801

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A variational method that involves solution of inhomogeneous linear equations is used to calculate the wave function and binding energy of the triton. Cohen and Willis's classification of the triton wave function is employed. Internal wave functions are expanded in terms of polynomials of the interparticle distances up to 170 terms. A binding energy of −6.7 MeV is obtained for the unmodified Hamada-Johnston potential. Due to the simplicity of our variational wave function, all the matrix elements are evaluated analytically in terms of the exponential integrals. With the aid of recurrence relations, the computing time has been reduced to a minimum.

I. INTRODUCTION

It is now quite clear that our knowledge of two-nucleon systems cannot give answers to all the problems of nuclear forces. Our next step is to look for some of the answers in the trinucleon system. We have sufficient experimental data for the ground states of the trinucleon systems. The recent data on charge and magnetic form factors by McCarthy *et al.*[1] are particularly revealing. We have not yet made sufficient use of such ground-state properties of the trinucleon system. In this article, we introduce a technique which is capable of calculating the ground-state properties of trinucleon systems with accuracy and efficiency.

Though our calculation is done with the Hamada-Johnston potential,[2] it can be extended to other potentials as well. Due to the simplicity of our variational wave function, simple recurrence relations can be found. In this calculation all the matrix elements are evaluated analytically in terms of the exponential integrals. The exponential integrals are evaluated with double-precision accuracy by a rational Chebyshev-polynomial approximation.[3]

A brief description of the spin-isospin and angular momentum part of the wave function is given in Sec. II. The variational method and the structure of the internal wave function are given in Sec. III. The convergence of the 170-term wave function is demonstrated in Sec. V. In Sec. VI, we give the results of the 170-term calculations with various components of the Hamada-Johnston potential, as well as with different values of the nonlinear variational parameter. Modification to the triplet odd quadratic spin-orbit potential[4] has not been included. All the energies are given in MeV and distances are given in units of the pion Compton wavelength.

II. TRITON GROUND-STATE WAVE FUNCTION

The ground state of the triton has total angular momentum $J=\frac{1}{2}$, isospin $T=\frac{1}{2}$, $T_3=-\frac{1}{2}$. Due to the presence of tensor and spin-orbit forces, it is a mixture of states with different orbital angular momentum, $l=0$, 1, 2. A detailed classification of the wave functions with various permutation properties is given by Cohen and Willis.[5] In our calculation, all the P states and the antisymmetric S states have been dropped. The wave functions included in our ground states are listed in Table I. We follow the notation used in Ref. 5, where the Y's are listed explicitly in terms of spin and isospin wave functions. In the D states, they also contain traceless second-rank tensors formed from the two vectors $\vec{r}$ and $\vec{\rho}$, where

$$\vec{r}=\sqrt{\tfrac{2}{3}}\,[\vec{R}_3-\tfrac{1}{2}(\vec{R}_1+\vec{R}_2)]\,,$$

$$\vec{\rho}=(1/\sqrt{2})\,(\vec{R}_2-\vec{R}_1)\,.$$

$\vec{R}_1$, $\vec{R}_2$, $\vec{R}_3$ are position vectors of the three nucleons relative to some fixed origin. The vectors $\vec{r}$, $\vec{\rho}$ and the interparticle distances r_{12}, r_{13}, r_{23} are shown in Fig. 1. The three nucleons are located at the corners of the triangle. It is clear that $\vec{r}$ and $\vec{\rho}$ determine uniquely the orientation, as well as the triangle itself. Therefore the orientation of the triangle need not be specified explicitly in terms of the Euler angles used in the classification of Derrick and Blatt.[6] The f's are the internal wave functions. They depend only on the interparticle distances r_{12}, r_{13}, r_{23}. Their structure will be discussed in Sec. III.

Our ground-state wave function is therefore

$$\psi=\psi_1+\psi_3+\psi_8+\psi_9+\psi_{10}+\psi_{11}\,, \tag{1}$$

which satisfies the equation

$$H\psi=E_0\psi\,. \tag{2}$$

E_0 is the ground-state energy and

$$H=-(\hbar^2/2M)(\nabla_r^2+\nabla_\rho^2)+\sum_{i<j}V(ij)\,. \tag{3}$$

M is the nucleon mass and V is the two-body Hama-

TABLE I. Basic eigenfunctions used in the ground state of H^3 ($J=\frac{1}{2}$, $J_M=\frac{1}{2}$, $T=\frac{1}{2}$, $T_3=-\frac{1}{2}$).

Eigenfunctions	Orbital angular momentum	Symmetry of the internal wave function f
$\psi_1=Y_1f_1$	S	Symmetric
$\psi_3=Y_{3,2}f_{3,1}-Y_{3,1}f_{3,2}$	S'	Mixed
$\psi_8=Y_8f_8$	D	Symmetric
$\psi_9=Y_9f_9$	D	Antisymmetric
$\psi_{10}=Y_{10,2}f_{10,1}-Y_{10,1}f_{10,2}$	D	Mixed
$\psi_{11}=Y_{11,2}f_{11,1}-Y_{11,1}f_{11,2}$	D	Mixed

da-Johnston potential.[2] It has central, tensor, spin-orbit, and quadratic spin-orbit components, each of which also depends on the spin and parity of the pair of nucleons involved. They are, respectively, ${}^3V_C^+$, ${}^3V_C^-$, ${}^1V_C^+$, ${}^1V_C^-$, ${}^3V_T^+$, ${}^3V_T^-$, ${}^3V_{LS}^-$, ${}^3V_{LS}^+$, ${}^3V_{LL}^+$, ${}^3V_{LL}^-$, ${}^1V_{LL}^+$, ${}^1V_{LL}^-$. Their values are taken from Table I of Ref. 2.

III. VARIATIONAL METHOD AND INTERNAL WAVE FUNCTIONS

The internal functions f are expanded in terms of simple polynomials of the interparticle distances with the appropriate symmetry. We have

$$f_i=e^{-\alpha(r_{12}+r_{13}+r_{23})}\Big\{\sum_{n_1,n_2,n_3\geq 1} a_{i,(n_1,n_2,n_3)} \times T\big[(r_{12}-r_0)^{n_1}(r_{23}-r_0)^{n_2}(r_{13}-r_0)^{n_3} \pm (r_{12}-r_0)^{n_1}(r_{13}-r_0)^{n_2}(r_{23}-r_0)^{n_3}\big]\Big\}. \tag{4}$$

i = 1, 3, 8, 9, 10, 11, the n's are positive integers greater than or equal to 1, and r_0 is the hard-core radius. T represents a group of symmetry operators defined by

$$T_S=(12)+(13)+(23),$$

$$T'=(\sqrt{3}/2)[(32)-(31)],$$

$$T''=(12)-\tfrac{1}{2}[(32)+(31)].$$

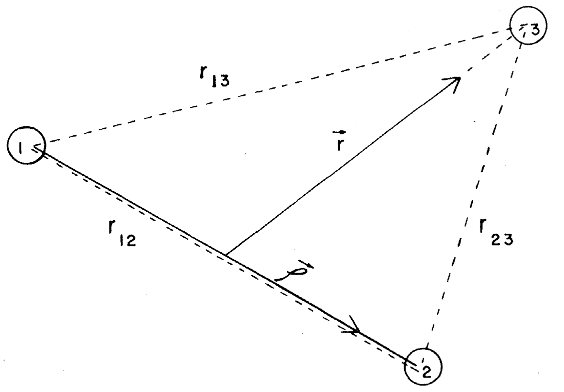

FIG. 1. Coordinates used in the triton wave function.

(12) represents the permutation of particles 1 and 2, etc. T_S gives the symmetric or antisymmetric f when used in (4) with the positive and negative signs, respectively. T' and T'' give the pair of mixed f's when used in (4) with the positive sign.

Let I represent the set of indexes i, n_1, n_2, n_3, and let N_I represent the normalization constant for the term denoted by I. We rewrite (4) as

$$f_{i\beta}=\sum_I A_I F_\beta(I). \tag{5}$$

The index β is absent except for mixed symmetric states where it takes the values 1 and 2.

$$F_\beta(I)=N_I e^{-\alpha(r_{12}+r_{13}+r_{23})} \times T\big[(r_{12}-r_0)^{n_1}(r_{23}-r_0)^{n_2}(r_{13}-r_0)^{n_3} \pm (r_{12}-r_0)^{n_1}(r_{13}-r_1)^{n_2}(r_{23}-r_0)^{n_3}\big].$$

The A_I are the linear variational parameters. α is a nonlinear variational parameter. Our variational method[7] requires the solution of the equation

$$(H-\lambda)\psi=\psi_0. \tag{6}$$

λ is a given parameter close to E_0, and ψ_0 is any given wave function not orthogonal to ψ. It turns out that for the kind of accuracy we need for the nuclear system, the choice of λ and ψ_0 is not very crucial. We choose ψ_0 to be one term in the symmetric S state.

When expansion (5) is substituted into (6), one can obtain a set of inhomogeneous linear equations in the unknown A_I. A set of solutions for A_I can readily be obtained, and a variational energy is given by

$$E_0\approx\int\psi^*H\psi\,de\Big/\int\psi^*\psi\,de.$$

The solution can be improved by repeating the above procedure with ψ_0 in (6) replaced by the solution ψ from the above step. The variational energy can be further improved by the method of moments.[7] However, the improvements from the last two steps are of relatively minor importance, whereas the total number of terms in the expansion is the only dominating factor in determining the variational solution of (2).

IV. EVALUATION OF COEFFICIENT MATRIX

We need to calculate the coefficient matrix

$$H_{IJ} = \sum_{\substack{\text{spin}\\ \text{isospin}}} \int_{\substack{\text{orientation}\\ \text{and interparticle}\\ \text{distances}}} F_\beta(I) Y_{i,\beta} H F_\gamma(J) Y_{j,\gamma}\, d\Omega \times r_{12} r_{13} r_{23}\, dr_{12}\, dr_{13}\, dr_{23}\,. \qquad (7)$$

The summations over the indices β and γ are specified according to Table I. The summation over spin and isospin and integration over orientation is done first to give

$$H'_{i\beta,j\gamma} = \sum_{\substack{\text{spin}\\ \text{isospin}}} \int_{\text{orientation}} Y_{i,\beta} H Y_{j,\gamma}\, d\Omega\,. \qquad (8)$$

$H'_{i\beta,j\gamma}$ are functions of interparticle distances only. The kinetic energy part of $H'_{i\beta,j\gamma}$ is identical to that given in Ref. 5. Due to the different structure of the Hamada-Johnston potential, the potential energy part of $H'_{i\beta,j\gamma}$ is not the same as that of Ref. 5, although it has the same general structure. For example, if one ignores the spin and parity dependence of the Hamada-Johnston potential, the spin-orbit part of $H'_{i\beta,j\gamma}$ reduces to that given in Ref. 5.

Substituting (8) into (7), we have

$$H_{IJ} = \int_{\substack{\text{interparticle}\\ \text{distances}}} F_\beta(I) H'_{i\beta,j\gamma} F_\gamma(J)\, r_{12} r_{13} r_{23}\, dr_{12}\, dr_{13}\, dr_{23}\,. \qquad (9)$$

The three interparticle distances are not all independent; they are required to satisfy the triangle relation throughout the integration. For most of the integrals, this is done by first integrating the

TABLE II. The exponents n_1, n_2, n_3 of the 170-term wave function.

Symmetric S and D			Mixed S' and D			Antisymmetric D		
n_1	n_2	n_3	n_1	n_2	n_3	n_1	n_2	n_3
0	0	0	1	0	0	0	1	2
1	0	0	1	0	1	0	1	3
1	0	1	2	0	0	0	1	4
1	1	1	2	0	1	0	2	3
2	0	0	2	0	2	0	2	4
2	0	1	2	1	1	0	3	4
2	0	2	2	1	2	1	2	3
2	1	1	3	0	0	1	2	4
2	1	2	3	0	1	1	3	4
2	2	2	3	0	2	2	3	4
3	0	0	3	0	3			
3	0	1	3	1	1			
3	0	2	3	1	2			
3	0	3	3	1	3			
3	1	1	3	2	2			
3	1	2	3	2	3			
3	1	3	4	0	0			
3	2	2	4	0	1			
3	2	3	4	0	2			
3	3	3	4	0	3			
4	0	0	4	0	4			
4	0	1	4	1	1			
4	0	2	4	1	2			
4	0	3	4	1	3			
4	0	4	4	1	4			
4	1	1	4	2	2			
4	1	2	4	2	3			
4	1	3	4	2	4			
4	1	4	4	3	3			
4	2	2	4	3	4			
4	2	3						
4	2	4						
4	3	3						
4	3	4						
4	4	4						

TABLE III. Binding energies and S-, S'-, D-state probabilties for the 170-term wave function with various components of the Hamada-Johnston potential.

α	E_0 $C+T$ (MeV)	P_S (%)	$P_{S'}$ (%)	P_D (%)	E_0 $C+T+LS$ (MeV)	P_S (%)	$P_{S'}$ (%)	P_D (%)	E_0 $C+T+LS+L_{12}$ (MeV)	P_S (%)	$P_{S'}$ (%)	P_D (%)
1.75	−2.47	93.33	0.10	6.57	−2.73	93.04	0.12	6.84	−0.946	93.74	0.17	6.09
2.00	−2.77	92.70	0.13	7.17	−3.10	92.38	0.16	7.46	−2.46	91.27	0.37	8.36
2.30	−2.82	92.12	0.14	7.74	−3.23	91.78	0.18	8.04	−4.47	88.94	0.43	10.63
2.50	−2.68	91.80	0.14	8.06	−3.13	91.45	0.18	8.37	−4.96	89.13	0.45	10.42
2.55	−2.62	91.72	0.14	8.14	−3.08	91.37	0.18	8.45	−5.15	88.95	0.45	10.60
2.60	−2.55	91.65	0.13	8.22	−3.03	91.30	0.17	8.53	−5.35	88.74	0.45	10.81
2.65	−2.48	91.57	0.13	8.30	−2.97	91.22	0.17	8.61	−5.55	88.49	0.46	11.05
2.70	−2.39	91.50	0.12	8.38	−2.89	91.15	0.17	8.68	−5.75	88.22	0.46	11.32
2.80	−2.19	91.35	0.12	8.53	−2.71	91.01	0.16	8.83	−6.17	87.54	0.46	12.00
2.90	−1.96	91.21	0.11	8.68	−2.50	90.87	0.15	8.98	−6.79	85.71	0.36	13.93
3.00	−1.69	91.07	0.10	8.83	−2.26	90.74	0.14	9.12	−5.87	86.81	0.86	12.33
3.20	−1.04	90.80	0.09	9.11	−1.64	90.48	0.12	9.40	−5.88	86.72	0.89	12.39

three variables independently outside the hard-core region, then subtracting those parts which do not satisfy the triangle condition. All the integrals then become elementary. With a combined use of recurrence relations and interchanging of the order of integrations, all the matrix elements may be evaluated analytically. One needs only to evaluate the exponential integrals

$$E_n(x), \quad n = 1, 2, 3, \ldots .$$

The normalization constants N_I and the overlapping integrals can be obtained by setting $H = 1$ in (7), (8), and (9). The largest coefficient matrix used in this calculation is 170× 170.

V. CONVERGENCE OF THE 170-TERM WAVE FUNCTION

The details of the structure of the 170-term wave function are given in Table II. n_1, n_2, n_3 are the powers of the polynomial defined in (4). Figure 2 gives plots of the binding energies, using only the central and the tensor part of the Hamada-Johnston potential, against the total number of terms included in the variational wave function. The successive points correspond to an increment of four terms in the symmetric states, three terms in the mixed symmetric states, and one term in the antisymmetric state in the order given in Table II. The upper curve corresponds to the Hamada-Johnston hard-core radius $r_0 = 0.343$. The lower curve corresponds to a 5% reduction in the hard-core radius with $r_0 = 0.326$. It is clear that both curves have sufficiently converged at 170 terms. The nonlinear parameter α is equal to 2 for both curves.

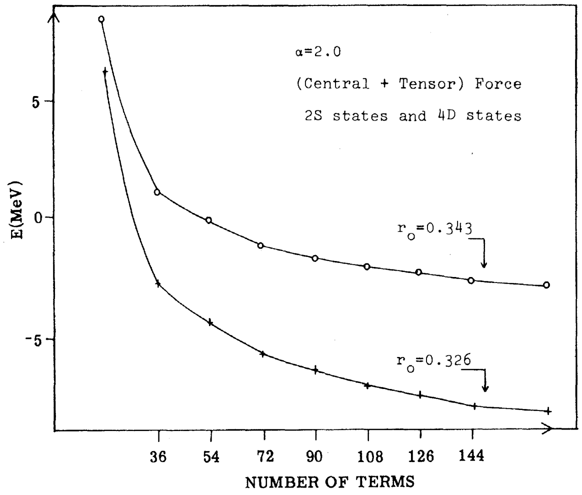

FIG. 2. Convergence of the binding energies as the total number of terms in the variational wave functions increases towards 170.

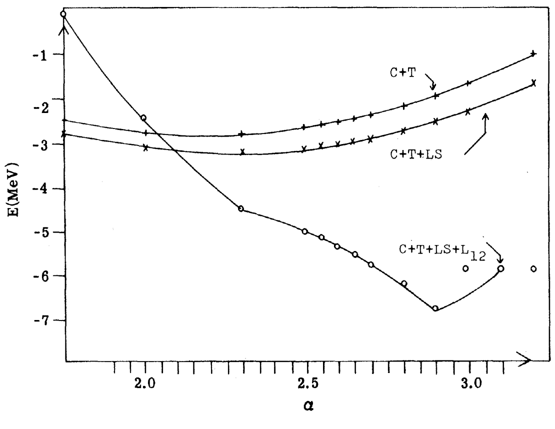

FIG. 3. Binding energies of the 170-term wave function with central + tensor, central + tensor + spin orbital, and central + tensor + spin-orbital + quadratic spin-orbital potential of the Hamada-Johnston potential, respectively, plotted against the nonlinear variational parameter.

VI. BINDING ENERGY OF THE HAMADA-JOHNSTON POTENTIAL

Using the 170-term wave function as given in Table II, Fig. 3 gives plots of the binding energies against the nonlinear variational parameter α. The curves correspond to central + tensor, central + tensor + spin-orbital, and the full Hamada-Johnston potential, respectively. The binding energies together with the corresponding S-, S'-, and D-state probabilities are given in Table III.

The binding energy of the full Hamada-Johnston potential has clearly reached a minimum at -6.7 MeV before numerical instability sets in at $\alpha > 3$. Although our calculation used double-precision programming, this numerical instability is caused by the loss of accuracy in applying the forward recurrence relation for the exponential integrals when some of the arguments of the exponential integrals are greater than 10. This situation will be corrected in our future calculation by using the recurrence relations more carefully. (There are existing techniques to take care of exponential integrals with large arguments.[8])

Table III gives the results of 12 runs. At present, each run takes 17 min. There is still room for improvement, since with additional use of disk storage the computing time can be reduced to less than 10 min. If more than one nonlinear parameter is used, the search for best nonlinear parameters can be done at a smaller number of terms in the linear parameter expansion.

VII. CONCLUSION

With one nonlinear variational parameter and 170 linear variational parameters we found a binding energy of -6.7 MeV for the triton, which is in agreement with that obtained by Delves *et al.*,[9] who have used a far more elaborate numerical technique. Our S'- and D-state probabilities differ considerably from their values of 1.8% and 9%, respectively. The primary source of these differences is that we have used the Hamada-Johnston potential[2] without the modification to ${}^3V_{LL}^{-}$. (In Delves *et al.*'s latest calculation this modification has been included.) It is expected that the wave function is far more sensitive to any change in the potential than is the binding energy. Secondly, we may have oversimplified our wave function in using only one nonlinear variational parameter for all states.

In this primary report, we give only the binding energies and the percentage of the various orbital angular momentum states. Many simple operators can easily be evaluated as by-products of the binding-energy calculation. The simplicity of our variational wave function can be very useful in calculating more-complicated ground-state properties such as the electric and magnetic form factors.

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