Microscopic calculations of ^{5}He with realistic interactions

J. Carlson
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

K. E. Schmidt and M. H. Kalos
Courant Institute of Mathematical Sciences, New York, New York 10012

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Microscopic calculations of low energy alpha neutron scattering are reported for the resonant $J^\pi = \frac{1}{2}^-$ and $\frac{3}{2}^-$ states. A good qualitative fit to the experimental $L\cdot S$ splitting is obtained, although discrepancies of the order of 1–2 MeV remain. Results with two different nucleon-nucleon interaction models are presented, and the effects of three-nucleon interactions are discussed.

I. INTRODUCTION

Microscopic calculations of nuclei with realistic interactions are very valuable in determining the extent to which nuclei may be successfully described as a system of nucleons. Many calculations of three- and four-body nuclei have been performed with realistic two- and three-nucleon interactions,[1–3] and the most recent calculations indicate that many of the properties of ^{3}He and ^{4}He can be correctly predicted with these models. Calculations of p-shell nuclei are important as a further test of these interactions. In particular, the negative parity components of the interaction are more important for these nuclei. In addition, the p-shell nuclei offer an opportunity to study $L\cdot S$ splittings in terms of these models.

In order to treat the heavier p-shell nuclei successfully, it is necessary to obtain a good variational description of the ^{5}He system. For example, the ^{6}He and ^{6}Li are very loosely bound, and previous calculations of these nuclei with three-body (alpha plus two nucleon) methods have been largely successful.[4] An accurate description of ^{5}He will presumably allow one to extend the calculations to heavier systems.

The ^{5}He system has been studied previously by several authors[5,6] who employ relativistic optical models in order to explain the magnitude of the splitting between the $J=\frac{1}{2}$ and $J=\frac{3}{2}$ states of alpha nucleon scattering. An important goal of this calculation is to determine to what degree the low energy splitting of these states can be explained using realistic two- and three-nucleon interactions in a nonrelativistic model.

The low energy $J=\frac{1}{2}$ and $\frac{3}{2}$ states of ^{5}He are calculated by converting the scattering problem into an equivalent bound state problem, as described in Ref. 7. Several enhancements to the method have been developed. These improvements reduce the computing time necessary to perform the variational calculations, and reduce the statistical error of the calculated phase shifts. In addition, they allow us to determine other quantities more accurately, such as the contribution of the different potential terms to the ^{5}He energy.

II. INTERACTION AND WAVE FUNCTION

The nuclear Hamiltonian used for these calculations has the form

$$\sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} \ , \tag{1}$$

where the two-nucleon interaction V_{ij} is given by

$$V_{ij} = \sum_k v^k(r_{ij}) O_{ij}^k \ . \tag{2}$$

The Reid soft core[8] interaction is written in terms of eight operators, including tensor and $L\cdot S$ interactions. We also report results for the more realistic Urbana V14 (Ref. 9) model, which contains 14 operators, including L^2 and $L\cdot S^2$ terms. The Urbana V14 interaction provides a better fit to the nucleon-nucleon phase shifts and deuteron properties.

The three-nucleon interaction used in this work is the Urbana model V. It may be written as a sum of two-pion exchange term $V^{2\pi}$ which is attractive in light nuclei, and an intermediate range repulsive term V^R. The more recent Urbana TNI model VII (Ref. 3) differs only in the magnitude of these components of the interaction. We include the expectation values of these terms separately, so that the model VII results may be obtained.

The wave function used for the ^{4}He and ^{5}He systems is given by the expression

$$\Psi = S\left[\prod_{i<j} F_{ij}\right]\Phi \ . \tag{3}$$

S indicates a symmetrization of the pair correlations, and Φ is a Slater determinant of one-body states coupled to the correct total angular momentum

$$\Phi = A\left\{\prod_i [\chi_\sigma(i)\chi_\tau(i)\phi(r_{i,\alpha})]\right\} \ . \tag{4}$$

A is an antisymmetrization operator and $r_{i,\alpha}$ is the distance from particle i to the system's center of mass in ^{4}He, and the distance to the center of mass of the four s-state particles in ^{5}He. The center of mass of the alpha particle in ^{5}He is different for different terms in the antisymmetrized Φ.

In previous calculations of s-shell nuclei, Φ was taken to be an antisymmetrized sum of spin states without any spatial dependence. The asymptotic form of the wave function as one particle is removed from the nucleus was built into the correlation operator. For p-shell nuclei, however, the differences between the asymptotic properties of the wave function as an s or p nucleon is removed

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are incorporated into the single particle term in the wave function.

The orbitals $\phi(r)$ are solutions of the Schrödinger equation in a Woods-Saxon well. The s-wave solutions are bound states of the well, and the p-shell orbital is a scattering state. The depth, radius, and skin thickness of the well are taken to be variational parameters, and may be different for the s and p orbitals in ^{5}He.

The pair correlation operators are obtained by solving the differential equations

$$-\frac{\hbar^2}{m}[\bar{\phi}\nabla^2 f_{S,T}+2\nabla\bar{\phi}\cdot\nabla f_{S,T}]+[\lambda_{S,T}+v_{S,T}]f_{S,T}\bar{\phi}=0 \tag{5}$$

in the singlet channels, and the coupled equations

$$-\frac{\hbar^2}{m}[\bar{\phi}\nabla^2 f_{S,T}+2\nabla\bar{\phi}\cdot\nabla f_{S,T}]+[\lambda_{S,T}+v_{S,T}]f_{S,T}\bar{\phi}+8v_{t,T}f_{t,T}\bar{\phi}=0\ , \tag{6}$$

$$-\frac{\hbar^2}{m}\left[\bar{\phi}\nabla^2 f_{t,T}+2\nabla\bar{\phi}\cdot\nabla f_{t,T}-\frac{6}{r^2}\bar{\phi}f_{t,T}\right]+[\lambda_{S,T}+v_{S,T}-2v_{t,T}-3v_{b,T}+6v_{q,T}+9v_{bb,T}]f_{t,T}\bar{\phi}+v_{t,T}f_{S,T}\bar{\phi}=0 \tag{7}$$

in the triplet channels.

The functions $f_{S,T}$ and $f_{t,T}$ are then cast into operator form so that

$$F(r_{ij})=f^c(r_{ij})\left[1+u_3\sum_k u_{ij}^k O_{ij}^k\right]\ . \tag{8}$$

f^c and u^k are obtained from Eqs. (5)–(7), and u_3 is the three-body correlation given in Ref. 10.

The boundary conditions imposed on the correlation functions require that the central correlation f^c go to one at a distance d, and the spin-isospin correlations u^σ, u^τ, and $u^{\sigma\tau}$ be zero for $r\geq d$. The tensor correlations have a long range. The functions $\bar{\phi}$ in the two-body equations are s and p wave radial functions in a harmonic oscillator potential. The strength of the oscillator and the distance d are variational parameters. Calculating the correlation in this way allows for a difference between the positive and negative parity pair correlations, in contrast to previous calculations of s shell nuclei. However, these correlations do not include $L\cdot S$ terms, and these terms may be important for ^{5}He. We hope to introduce them in future calculations.

III. CALCULATIONS

The low energy phase shifts in a one channel scattering problem may be determined by converting it into an equivalent bound state problem.[7] This method is particularly suited to the calculation of low energy resonances, such as the $J=\frac{1}{2}$ and $\frac{3}{2}$ states of ^{5}He. If the two scattering products are confined to a region such that the distance between them is less than a distance R_n, and the Schrödinger equation is solved in this region with the boundary condition that the wave function be zero at the boundary, the phase shift δ_l is given by

$$\tan(\delta_l)=\frac{j_l(kR_n)}{n_l(kR_n)}\ , \tag{9}$$

where

$$k=[2\mu E_{\rm sep}/\hbar^2]^{1/2}\ . \tag{10}$$

In these equations, μ is the reduced mass and j_l and n_l are spherical Bessel functions. $E_{\rm sep}$ is the separation energy, defined as the difference between the total energy of the system confined within the box and the sum of the energies of the separated products. This method requires R_n to be large enough so that the potential acting between the systems is zero when they are separated by a distance greater than or equal to R_n. For this reason it is most useful for low energy scattering. Boundary conditions other than $\Psi(R_n)=0$ may be employed, and Eq. (9) altered appropriately.

We use the Metropolis Monte Carlo method to calculate the energies of light nuclei.[10] This method allows one to obtain a set of configurations distributed in coordinate space with a probability density proportional to the square of the variational wave function. For light nuclei, all spin-isospin states of the wave function are calculated at each step of the random walk. The expectation value of the Hamiltonian is determined by summing over all spin-isospin states at each point and then taking the average over all configurations.

In order to calculate the phase shift with this method, the separation energy $E_{\rm sep}$ must be accurately determined. $E_{\rm sep}$ is the difference between the ^{5}He and alpha particle energies. Each of these energies is subject to the statistical error associated with Monte Carlo integration. For this system the error is dominated by the energy of the four s shell nucleons, since they occupy a much smaller volume than the p shell nucleon.

The energy difference $E_{\rm sep}$ may be calculated directly in order to reduce the statistical error. We calculate the difference by writing

$$E(^4\mathrm{He})=\frac{\int dr_1\cdots dr_5\Psi_4^\dagger(1,2,3,4)H_4\Psi_4(1,2,3,4)G(\mathbf{r}_{5,\alpha})}{\int dr_1\cdots dr_5\Psi_4^\dagger(1,2,3,4)\Psi_4(1,2,3,4)G(\mathbf{r}_{5,\alpha})}\ , \tag{11}$$

where Ψ_4 is the alpha particle wave function and H_4 is the Hamiltonian acting on nucleons 1–4. If G is a function of the vector from r_5 to the center of mass of the alpha particle, the integrations over r_5 cancel and we are left with the usual expression for the energy of the alpha particle.

Rewriting the energy in this way is useful because it allows us to use the same set of configurations to calculate the energy of both ^{5}He and the alpha particle. If we have a set of points R_i distributed with probability density

$$W(r_1 \cdots r_5)=\Psi_5^\dagger(r_1 \cdots r_5)\Psi_5(r_1 \cdots r_5) ,$$

both the numerator and denominator of Eq. (11) may be multiplied by W, and the energy of the alpha particle is given by

$$E(^4\text{He})=\frac{\sum \frac{\Psi_4^\dagger H_4 \Psi_4}{\Psi_4^\dagger \Psi_4}\frac{\Psi_4^\dagger \Psi_4 G_{5,\alpha}}{W}}{\sum \frac{\Psi_4^\dagger \Psi_4 G_{5,\alpha}}{W}} . \tag{12}$$

The sums in Eq. (12) run over the set of points $\{R_i\}$ generated in the random walk.

In order to minimize the variance, we choose

$$G_{5,\alpha}=[\phi^\dagger(r_{5,\alpha})\phi(r_{5,\alpha})]\Theta(R_{5,\alpha}-R_0) , \tag{13}$$

where ϕ is the single particle wave function in the p-wave state. This choice leads to a low variance because each term in the denominator of Eq. (12) is near 1. In the limit of two noninteracting reaction products, this method will give $E_{\text{sep}}=0$ with zero variance. The Θ function is included in $G_{5,\alpha}$ so that those configurations in which all the particles are close together do not contribute to the expectation value in ^{4}He. This is necessary to prevent large fluctuations when particle 5 is near one of the other particles.

The energy of ^{5}He may be determined from the same set of configurations in the usual manner:

$$E(^5\text{He})=\frac{\sum \frac{\Psi_5^\dagger H_5 \Psi_5}{W}}{\sum \frac{\Psi_5^\dagger \Psi_5}{W}} . \tag{14}$$

The statistical error in the difference $E(^5\text{He})-E(^4\text{He})$ is significantly less than that obtained from two independent Monte Carlo calculations. The computer time required for a given variance will be reduced by a factor from 5 to 15, depending upon the state being calculated and the value of R_n. It is also very useful to minimize the variational energy of ^{5}He by reweighting a set of configurations rather than performing independent calculations. Energy differences may easily be determined within 0.1 to 0.2 MeV in this manner.

IV. RESULTS

The first step in determining the phase shifts of ^{5}He is to calculate the binding energy of ^{4}He. This calculation provides a significant test of our parametrization of the alpha particle wave function. For the Urbana V14 + TNI V interaction, we obtain an energy of -29.6 ± 0.3 MeV, which is consistent with previous calculations using a different parametrization. The alpha particle is slightly over bound with this interaction, but this should not strongly affect the alpha neutron scattering energy.

The results of our calculations of the $J=\frac{1}{2}$ and $\frac{3}{2}$ ^{5}He scattering states are summarized in Table I and Figs. 1 and 2. Figure 1 presents the calculated and experimental[11] phase shifts for both the $J=\frac{1}{2}$ and $\frac{3}{2}$ states, for the Urbana V14 plus TNI V interaction model. The equivalent information is presented in Fig. 2 as a plot of the separation energy E_{sep} vs R_n. In the second figure, the dashed line represents the energy for a free nucleon confined within R_n, the solid lines give the experimental results, and the points with error bars are the results of our calculations. Both the Urbana and Reid two-nucleon interaction results are presented in this figure.

For the Urbana V14 + model V TNI, the $J=\frac{1}{2}$ energies are approximately 1 MeV too high at small R_n, while the $J=\frac{3}{2}$ energies are approximately 2 MeV too large. Thus, we obtain a splitting between the two states which is somewhat smaller than the experiment would indicate. Nevertheless, we obtain roughly 80 percent of the difference between the free particle solution and the experimental $J=\frac{3}{2}$ result at $R_n=5.5$ fm, and approximately three-fourths of the experimental splitting between the two states.

The total energy and the contributions of various potential terms are presented in Table I. The ^{5}He results are given for $R_n=7.5$ fm. The first row gives the expectation values for the alpha particle, and the second and third rows give the additional contribution in the $J=\frac{1}{2}$ and $\frac{3}{2}$ ^{5}He states, respectively. These differences are obtained with the same subtraction technique used for the total energy.

The orbitals used for the two ^{5}He states are different in these calculations, so we have also calculated a "perturba-

TABLE I. The total energy and contributions of the Urbana V14 plus TNI model V interaction for ^{4}He and ^{5}He. The complete energy and potential energy are given for the alpha particle, while in ^{5}He the alpha particle contributions are subtracted. R_n is 7.5 fm. The last row gives the perturbative difference between the two ^{5}He states (see the text).

State	$\langle H \rangle$	$\langle V_{ij} \rangle$	$\langle V_{ijk}(2\pi) \rangle$	$\langle V_{ijk}(R) \rangle$
^{4}He	-29.6 ± 0.3	-136.0 ± 2.0	-10.4 ± 0.4	3.9 ± 0.2
^{5}He ($J=\frac{3}{2}$)	4.2 ± 0.2	-14.0 ± 1.2	-0.9 ± 0.2	0.5 ± 0.1
^{5}He ($J=\frac{1}{2}$)	6.5 ± 0.2	-6.0 ± 1.0	-0.2 ± 0.1	0.2 ± 0.1
Difference	3.1 ± 0.3	5.4 ± 1.5	0.7 ± 0.3	-0.1 ± 0.1

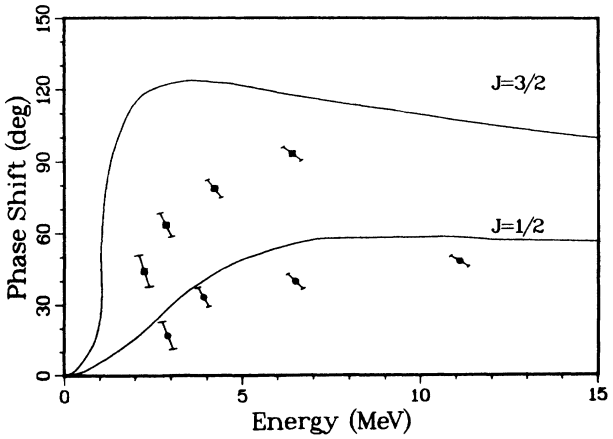

FIG. 1. Phase shifts versus energy for $J=\frac{1}{2}$ and $\frac{3}{2}$ alpha neutron scattering. The solid curves give the experimental results, while the points with error bars indicate the calculated results and statistical errors for the Urbana V14 + TNI V interaction.

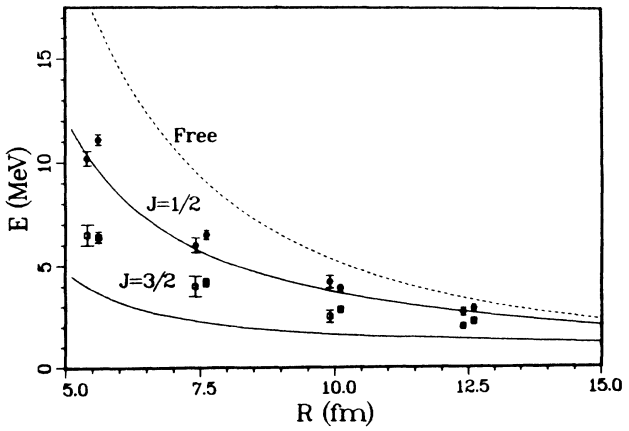

FIG. 2. Energy versus confinement radius R_n for ^{5}He. The dashed line indicates the energy of a noninteracting nucleon confined within R_n, and the solid lines are obtained from the experimental phase shifts. The open and closed symbols represent calculated results for the Urbana V14 and Reid interactions, respectively. Both calculations include the Urbana model V TNI. The calculated points have been shifted slightly for clarity.

tive" energy difference between the two states. In this calculation, we used the same single particle orbitals and pair correlations for both states. The only difference between the wave functions is the angular momentum coupling. Subtracting the expectation values in the two states gives the contributions of different interaction terms to the splitting. These contributions are listed in the last row of Table I. These perturbative wave functions give total energies not very different from the optimum variational wave functions.

It is apparent from these results that most of the splitting arises from the two-nucleon interaction, primarily from the $L\cdot S$ terms. The two pion exchange three-nucleon interaction does contribute roughly 0.7 MeV, however. The three-nucleon interaction has a somewhat larger effect at smaller R_n (higher energy). The results plotted in Fig. 2 for the Reid interaction are slightly different than those obtained in Ref. 12. This is due to the use of an incorrect (weaker) short range cutoff of the three-nucleon interaction in the earlier work. In addition, the Monte Carlo calculations have been lengthened to further reduce the statistical errors.

V. CONCLUSIONS

These calculations suggest that a substantial fraction of the splitting between the $J=\frac{1}{2}$ and $J=\frac{3}{2}$ states in alpha neutron scattering may be explained in a microscopic nonrelativistic treatment with realistic interactions. We obtain roughly three-fourths of the correct splitting at $R_n=5.5$ fm and 80% of the difference between the free particle case and the experimental results for the $J=\frac{3}{2}$ state. Thus, a good qualitative picture of alpha neutron scattering is obtained, but there are disagreements with experiment in both the overall attraction and the $L\cdot S$ splitting at the 1–2 MeV level.

These differences are roughly comparable to a previous calculation of the excited states of the alpha particle.[7] It is not clear whether the variational wave function is general enough to give the energy to the desired accuracy, or if the interaction itself is inadequate. An obvious choice for the improvement of the wave function would be to introduce $L\cdot S$ pair correlations. Although this is technically difficult because of the derivatives involved, results with this more general wave function would help to determine the cause of the remaining differences.

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[1]J. Carlson, V. R. Pandharipande, and R. B. Wiringa, Nucl. Phys. **A401**, 59 (1983).
[2]C. R. Chen, G. L. Payne, J. L. Friar, and B. F. Gibson, Phys. Rev. C **33**, 1740 (1986).
[3]R. Schiavilla, V. R. Pandharipande, and R. B. Wiringa, Nucl. Phys. **A449**, 219 (1986).
[4]D. R. Lehman and W. C. Parke, Phys. Rev. Lett. **50**, 98 (1983).
[5]L. G. Arnold, B. C. Clark, R. L. Mercer, D. G. Ravenhall, and A. M. Saperstein, Phys. Rev. C **14**, 1878 (1976).
[6]L. G. Arnold, B. C. Clark, and R. L. Mercer, Phys. Rev. C **19**, 917 (1979).
[7]J. Carlson, V. R. Pandharipande, and R. B. Wiringa, Nucl. Phys. **A424**, 427 (1984).
[8]R. V. Reid, Ann. Phys. (N.Y.) **50**, 411 (1968).

[9]I. E. Lagaris and V. R. Pandharipande, Nucl. Phys. **A355**, 331 (1981).
[10]J. Lomnitz Adler, V. R. Panharipande, and R. A. Smith, Nucl. Phys. **A361**, 339 (1981).
[11]R. A. Arndt and L. D. Roper, Nucl. Phys. **A209**, 447 (1973).
[12]J. Carlson, K. E. Schmidt, and M. H. Kalos, in *Condensed Matter Theories,* edited by F. B. Malik (Plenum, New York, 1985), Vol. I, p. 79.