Cluster Model Calculation on the Energy Levels of the Lithium Isotopes*

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A variational procedure is adopted to determine the energies of the levels of the highest space symmetry type in Li^6 and Li^7. The trial wave functions employed take into consideration the existence of cluster structures in those nuclei. With a simple two-body force, it is shown that the computed energies of the various states are in reasonable agreement with experiment. The $^2F_{\frac{5}{2}}$ level in Li^7, as yet undetermined experimentally, is found to have an excitation energy of about 5.6 Mev and a rather large level width. The calculation also indicates that to explain the splitting of levels in those nuclei, a constant two-body spin-orbit force of the pure neutral form is inadequate.

I. INTRODUCTION

IN two previous papers[1,2] (hereafter referred to as I and II), we have examined the behavior of the low-lying levels in Be^8, Li^7, and He^5 within the framework of the cluster model.[3] The results obtained were generally quite encouraging. In addition to producing a satisfactory fit to the energies of the various levels, the model also presented a qualitative picture of the level widths as well as a unique means of labeling these levels, i.e., parity, angular momentum, etc. In this paper, we continue the study by investigating the nucleus Li^6, with the hope that with the same two-body force as previously employed, we can obtain good agreement with the experimental binding energies.

In addition, we have re-examined the nuclei Li^7 and Be^7 with a three-parameter variational wave function. Inasmuch as we desire to determine the energies of all levels of the space symmetry type [3], a spin-orbit term of the type introduced in II is also incorporated in our two-body force. The reasons for refining the calculation in I in the manner described are twofold. First, it is of major interest to determine whether the additional variational parameter drastically affects our results and, second, it would be interesting to understand why the $(\frac{5}{2}-)$ level of the ^2F doublet has so far escaped detection, if indeed it exists at all.[4] It is quite certain now that the $(\frac{5}{2}-)$ level at[5] 7.47 Mev in Li^7 is of the term $^4P_{\frac{5}{2}}$ and hence, is not a member of the ^2F doublet.[6] Meshkov and Ufford[7] inferred from the spectra of Li^6 that this latter level ($^2F_{\frac{5}{2}}$) should lie somewhere around 6.5 Mev, whereas Marion[8] speculated that the difficulty in detecting this level experimentally can probably be attributed to a large level width. Since our calculation presents a rough estimate of level widths, we are thus encouraged to re-examine these nuclei in greater detail.

The level structure of Li^6 and Li^7 and all other p-shell nuclei has been extensively studied by Inglis[9] and Kurath[10] in the intermediate-coupling picture. By varying essentially only two parameters, the exchange energy integral and the intermediate-coupling parameter, these authors showed that the level schemes of the p-shell nuclei can be fairly well reproduced. From a fundamental point of view, however, it seems more desirable to calculate both the binding energies and the level spacings from the two-body interaction directly. To date, several authors[11] have attempted such a calculation; however, their method was restricted in the sense that they incorporated only the lowest shell model configurations, i.e., $(1s)^4(1p)^n$. More realistically, the wave function should not be limited to those configurations in which all nucleons outside of the closed shells are in the energetically lowest, incomplete shell. Rather one must employ fairly accurate wave functions, and this certainly implies mixing of many excited configurations. This latter view is indeed supported by the work of Feingold[12] and Lyons[13] on the level scheme of Li^6 and by our work on He^5 and Li^5.[2]

Our basic aim is, therefore, to calculate the energies of the various low-lying levels in Li^6 and Li^7 by using information about the nucleon-nucleon interaction as

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[1] L. D. Pearlstein, Y. C. Tang, and K. Wildermuth, Nuclear Phys. **18**, 23 (1960); Bull. Am. Phys. Soc. **4**, 271 (1960).

[2] L. D. Pearlstein, Y. C. Tang, and K. Wildermuth, Phys. Rev. **120**, 224 (1960).

[3] K. Wildermuth and T. Kanellopoulos, Nuclear Phys. **7**, 150 (1958); **9**, 449 (1958/1959); CERN Rept. 59-23.

[4] *Proceedings of the International Conference on Nuclear Structure, Kingston*, edited by D. A. Bromley and E. W. Vogt (University of Toronto Press, Toronto, Canada, 1960), p. 417.

[5] All experimental data are taken from the compilation of F. Ajzenberg-Selove and T. Lauritsen, Nuclear Phys. **11**, 1 (1959).

[6] J. M. Soper, Phil. Mag. **2**, 1219 (1957); J. B. French and A. Fujii, Phys. Rev. **105**, 652 (1957).

[7] S. Meshkov and C. W. Ufford, Phys. Rev. **101**, 734 (1956).

[8] J. B. Marion, Nuclear Phys. **4**, 282 (1957).

[9] D. R. Inglis, Phys. Rev. **87**, 915 (1952); Revs. Modern Phys. **25**, 390 (1953).

[10] D. Kurath, Phys. Rev. **101**, 216 (1956).

[11] M. Morita and T. Tamura, Prog. Theoret. Phys. (Kyoto) **12**, 653 (1954); J. Irving and D. S. Schonland, Phys. Rev. **97**, 446 (1955); J. P. Elliott, Proc. Roy. Soc. (London) **A218**, 345 (1953).

[12] A. M. Feingold, Phys. Rev. **101**, 258 (1956).

[13] D. H. Lyons, Phys. Rev. **105**, 936 (1957).

deduced from data on the two-body system directly. We shall employ a variational method, with the wave functions prescribed by the cluster model recently proposed.[3,14] As the basic ideas of this model have already been discussed elsewhere,[3] we shall not describe it here. It suffices only to mention that experimental evidence for the presence of cluster structures in light- and medium-weight nuclei seems to be rather abundant.[15] This model is especially suited for calculation in light nuclei, since it is formulated in such a manner as to present an obvious correspondence between certain experimental facts and a particular eigenfunction of a complete cluster wave-function system. Namely, consider a state of a nucleus which decays primarily into two composite particles, a prudent description of this system would be the proper two-clusters configuration, with the actual details being determined by the relative motion engaged in by the two clusters. Of course, the suitable choice of cluster wave-function system can change from level to level.[16,17] For instance, for He^5 it is found in II that for the ground and first excited states, an alpha cluster plus a neutron representation is most suitable for their description, while for the state at 16.69 Mev excitation, a triton cluster plus a deuteron cluster representation would be more convenient, since in their appropriate representations, the states can be described essentially by a single antisymmetrized cluster wave function. As to the question of how to choose the most appropriate cluster function system for a particular level—one must normally employ a trial-and-error procedure, although, in many cases, insight can be gained by studying experimental information about the level, such as its reduced width for a particular decay channel, its Coulomb energy behavior,[18] and so on.

Also of interest is the question as to what is the exact form of the two-body spin-orbit force. Specifically, can a neutral spin-orbit force adequately explain the level splittings in all light nuclei or is it necessary to include a symmetric component?[19] By an analysis of single-particle and single-hole splittings in He^5 and N^{15},[20] Elliott and Lane have shown that the neutral form is presumably the more appropriate one. On the other hand, Abraham[21] concluded from the ^2P splitting in Li^7 that the symmetric term must also play an important role. These contradictory conclusions, however, were based on a simple shell model calculation with a configuration $(1s)^4(1p)^n$. Since our $He^5(Li^5)$ calculation indicated that the effect of mixing in higher configurations is quite significant, the conclusions of the above authors may be considerably modified by this latter complication. Thus, there remains the definite need to determine whether a constant two-body neutral spin-orbit force can successfully account for all the spin-orbit splittings in He^5, Li^6, and Li^7.

In the next section, a brief description of the two-body force and of the method of calculation will be presented. Sections III and IV are devoted to the explicit calculations of Li^6 and Li^7, respectively. In this investigation, we have only considered levels of the highest space symmetry type, i.e., $[\lambda]=[3]$ for Li^7 and $[\lambda]=[2]$ for Li^6. Finally, in Sec. V, we summarize and discuss the results of the present investigation, together with results taken from I and II on He^5 and Be^8. Also, in this section, a rough indication of how to extend our method of calculation to heavier nuclei is presented.

II. METHOD OF CALCULATION

The procedure for evaluating the energy of a level has been discussed in I and II; hence, we shall present only a brief review here. We compute the energy by the usual Ritz variational method; that is, we minimize the expression

$$E=\int \Psi^* H\Psi d\tau \Big/ \int \Psi^*\Psi d\tau, \tag{1}$$

with respect to all parameters in the variational wave function Ψ. In Eq. (1), H is the Hamiltonian operator and has the form

$$H=(-\hbar^2/2M)\sum_{\text{all particles}}\nabla_i^2+\sum_{\text{all pairs}}V_{ij}, \tag{2}$$

with V_{ij} being the two-body potential.

For the computation of E, one should certainly use a realistic two-body force with hard core. However, to compute with such a force would be a nearly prohibitive procedure; therefore, we shall in this investigation use an approximation method which simplifies calculations greatly. Essentially, what we do is to separate the total energy into two parts, one part pertaining to the internal energies of the clusters and the other part relating to the interaction energy between the clusters. To compute the interaction energy, we make the assumption that since the clusters in a light nucleus would normally be quite far apart, we can compute it by employing a simple two-body force of nonsaturating character, but one which is in accord with all low-energy two-nucleon phenomena.[22] As for the internal energies,

[14] The ideas of the cluster model are basically similar to those of the resonanting-group method devised by J. A. Wheeler [Phys. Rev. **52**, 1083, 1107 (1937)].

[15] R. K. Sheline and K. Wildermuth, Bull. Am. Phys. Soc. **5**, 271 (1960); B. Roth and K. Wildermuth, Nuclear Phys. **20**, 10 (1960).

[16] Theoretically one can use a single eigenfunction system, for instance the single-particle shell model eigenfunction system, to describe the behavior of all nuclear levels. Often, however, the description becomes very complicated and also physical insight into the problem is frequently lost.

[17] For connections between cluster function system and the single-particle eigenfunction system, see J. K. Perring and T. H. R. Skyrme, Proc. Phys. Soc. (London) **A69**, 600 (1956); D. M. Brink, Nuclear Phys. **4**, 215 (1957); T. Kanellopoulos and K. Wildermuth, *ibid.* **14**, 349 (1959/1960).

[18] K. Wildermuth and Y. C. Tang, Phys. Rev. Letters **6**, 17 (1961).

[19] J. P. Elliott and A. M. Lane, *Encyclopedia of Physics*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 39, p. 331.

[20] J. P. Elliott and A. M. Lane, Phys. Rev. **96**, 1160 (1954).

[21] G. Abraham, Nuclear Phys. **1**, 415 (1956).

[22] Since we include only central forces, the static moments of the deuteron, of course, cannot be properly reproduced.

it is assumed that the same simple force will suffice for the deuteron cluster case, while for the cases of the alpha and triton clusters, a more realistic force with hard core should really be used. In this work, instead of actually computing the internal energies of the latter clusters, we use experimental information about the three- and four-body bound systems and infer the compressibilities of the clusters from a calculation of Mang and Wild.[23] The explicit expressions for the internal energies of the alpha and triton clusters as a function of their cluster sizes will be given in the next section.

Since the present investigation is of an exploratory nature, we shall use a very simple Serber force which fits the two-nucleon data to about 40 Mev to compute the interaction energy. It has the following form[24]:

$$V_{ij}=-V_0\exp(-\kappa r_{ij}^2)\{w(1+P_{ij}^r)+b(P_{ij}^\sigma-P_{ij}^\tau)\}-V_{LS}\exp(-\lambda r_{ij}^2)(\mathbf{r}_i-\mathbf{r}_j)\times(\mathbf{p}_i-\mathbf{p}_j)\cdot(\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_j)\hbar^{-1}/2+e^2\epsilon_{ij}/r_{ij}, \quad (3)$$

with $\epsilon_{ij}=1$ if i, j are protons and 0 otherwise. In Eq. (3), $V_0=68.6$ Mev, $\kappa=4.16\times10^{25}$ cm^{-2}, $w=0.41$, $b=0.09$, and P_{ij}^r, P_{ij}^σ, P_{ij}^τ represent the space, spin, and isobaric spin exchange operators, respectively. The range λ and depth V_{LS} of the neutral spin-orbit potential will be discussed when the results of our calculations are presented.

III. ENERGY LEVELS OF Li^6

A. Qualitative Description

For the discussion of the spectrum of Li^6, it is proper to choose an alpha cluster plus a deuteron cluster representation. The wave functions of this representation have the symbolic form

$$\Psi=A\{\Phi_j(\alpha)\Phi_k(d)\chi(\mathbf{R}_\alpha-\mathbf{R}_d)\}, \quad (4)$$

where $\Phi_j(\alpha)$ and $\Phi_k(d)$ refer to wave functions which describe an alpha-cluster in its jth state and a deuteron cluster in its kth state, respectively, and $\chi(\mathbf{R}_\alpha-\mathbf{R}_d)$ pertains to the relative motion between the alpha and the deuteron clusters. The operator A signifies the complete antisymmetrization of the wave function with respect to the exchange of all pairs of particles.

We begin by describing the triplet states of Li^6 ($T=0$, $S=1$) with excitation energies less than 6 Mev. For those levels, a description with unexcited alpha cluster and triplet deuteron cluster should be adequate. Since in the single-particle shell model picture, two nucleons are in the $1p$ shell, the relative oscillation function $\chi(\mathbf{R}_\alpha-\mathbf{R}_d)$ must be of second order with $L=0$ or 2 in accordance with the Pauli exclusion principle. The $L=0$ configuration should give rise to the lowest state, since in this configuration, the clusters are, on the average, closer to each other. Thus, the ground state of Li^6 has the assignment (1^+) in agreement with experimental finding. On the other hand, since there is a spin-orbit potential, the degenerate $L=2$ states are split into three states with $J=3$, 2, 1, with the $J=3$ state having the lowest energy. This is again the observed level sequence. We like to mention here that the description of these $T=0$ states by the assumed configurations finds strong support from the experimentally determined values of reduced level widths. It was found that for all those $L=2$ levels, the reduced widths leading to the decay into a deuteron and an alpha particle are in the neighborhood of the Wigner limit, suggesting a high degree of $\alpha-d$ configuration in the wave functions.[25]

Now we consider the singlet states of Li^6 ($S=0$, $T=1$) with excitation energies less than 6 Mev. Here $\chi(\mathbf{R}_\alpha-\mathbf{R}_d)$ must again describe motion of the alpha cluster relative to the singlet deuteron cluster with orbital angular momentum 0 and 2. But in the singlet case, since the deuteron cluster has zero spin angular momentum, there is only one state for each value of L. Therefore, the only low-energy singlet levels of Li^6 with excitation energies less than about 6 Mev are the $J=0$ and $J=2$ levels, which is again in complete agreement with experiment.

In the above discussion and the ensuing quantitative treatment, we have assumed that all the levels can be described by a pure configuration in the cluster wave-function system; in other words, we have adopted, in first approximation, the $L-S$ coupling scheme by assuming that both L and S are good quantum numbers. With the inclusion of a spin-orbit term in our two-body force, it is of course well-known that neither S nor L is good. Thus, our assumption of a pure configuration can only be approximately valid. For instance, for the ground state of Li^6, the spin-orbit term mixes the state $^3S_1$ with the states $^3D_1$ and $^1P_1$. However, it has been shown that for nuclei in which a new shell has just been started, the $L-S$ coupling scheme should represent a fairly good approximation.[10] For Li^6, further support in favor of the $L-S$ model can also be found in the comparison between the theoretically calculated and experimentally observed values of the magnetic moment and quadrupole moment.[11] Thus, our simplifying assumption of a pure configuration in our trial wave function should introduce a relatively small error into our calculation.

We would speculate that the group of levels at 6.63, 7.40, 8.37, and 9.3 Mev[5] arise from the motion of an alpha cluster relative to a two-nucleon system in an internal p state. Then in our picture, $\chi(\mathbf{R}_\alpha-\mathbf{R}_d)$ would be of first order with $L=1$, and those four levels can be identified with the assignment $^3P_2$, $^1P_1$, $^3P_1$, and $^3P_0$. From the fact that two nucleons interact very weakly in a relative p state if a two-body force of the form (3) is assumed, we can easily estimate in a rough manner the approximate location of these levels on the energy scale by considering the experimental binding energies of He^5

[23] H. J. Mang and W. Wild, Z. Physik **154**, 182 (1959). For a discussion of the applicability of their results to our calculations, see II.

[24] K. Lederer, Diplomarbeit, Munchen, 1957 (unpublished).

[25] A. Galonsky and M. T. McEllistrem, Phys. Rev. **98**, 590 (1955).

and Li^5 relative to that of an alpha particle plus a free nucleon. Such a rough estimate yields the value 6.6 Mev, indicating that our assumed configuration for this group of levels is probably correct.

From our calculations in I and II, we can also predict that the alpha-deuteron configuration in relative $3p$ and $3f$ states cannot properly describe resonant states. Thus, the levels recently reported to lie around 12.5 Mev[26] should be described by a configuration in which the alpha cluster is broken up.

B. Quantitative Treatment

As mentioned in the Introduction, we shall calculate only the energies of those levels with the highest space symmetry, i.e., the first six levels of Li^6. The group of levels at about 7 and 12.5 Mev will not be quantitatively treated in this investigation.

For the trial wave function, we choose

$$\Psi=A\{\psi(1234;56)\xi(1234;56)\}$$
$$=A\left\{\exp\left(-\frac{\alpha}{2}\sum_{i=1}^{4}\rho_i^2\right)\exp\left(-\frac{\bar{\alpha}}{2}\sum_{j=5}^{6}\rho_j^2\right)\right.$$
$$\left.\times R^n Y_{LM}(\mathbf{R}/R)\exp(-\tfrac{2}{3}\beta R^2)\xi(1234;56)\right\}, \quad (5)$$

where $\xi(1234;56)$ is a charge-spin function, and $\psi(1234;56)$ denotes the space part of the wave function written in the notation of Edwards.[27] This notation simply means that ψ describes particles 1, 2, 3, 4 in the alpha cluster and 5, 6 in the deuteron cluster. Also in Eq. (5),

$$\boldsymbol{\rho}_i=\mathbf{r}_i-\mathbf{R}_\alpha, \quad \boldsymbol{\rho}_j=\mathbf{r}_j-\mathbf{R}_d, \quad (6)$$

and

$$\mathbf{R}=\mathbf{R}_\alpha-\mathbf{R}_d, \quad (7)$$

with

$$\mathbf{R}_\alpha=\tfrac{1}{4}\sum_{i=1}^{4}\mathbf{r}_i, \quad \mathbf{R}_d=\tfrac{1}{2}\sum_{j=5}^{6}\mathbf{r}_j. \quad (8)$$

Our particular choice of the wave function is dictated by our desire that when $\alpha=\bar{\alpha}=\beta$, it reduces to the usual shell model function describing the lowest configuration $(1s)^4(1p)^2$ in an oscillator potential well of width parameter α.

The particular choice of n and L in the trial wave function has been explained in detail in Sec. III A; that is, $n=2$, $L=0$ for states with terms $^3S_1$, $^1S_0$, and $n=2$, $L=2$ for states with terms $^3D_3$, $^3D_2$, $^3D_1$, $^1D_2$.

The method of computing the expectation value of the Hamiltonian operator has been discussed in I and II; hence, we shall present here only the general form of the results, while listing the various potential integrals in the Appendix. The normalization factor N^2, kinetic energy $\langle T\rangle$ and potential energy $\langle V\rangle$ can be easily shown to have the following forms:

$$N^2=6!\int(\psi_0-2\psi_1+\psi_2)^*\psi_0 d\tau, \quad (9)$$

in which

$$\psi_0=\psi(1234;56),$$
$$\psi_1=\psi(5234;16), \quad (10)$$
$$\psi_2=\psi(5634;12),$$

with the subscripts 0, 1, 2 denoting no-exchange, one-exchange, and two-exchange, respectively.

$$\langle T\rangle=(\hbar^2/2M)(2n\beta+3\beta+9\alpha+3\bar{\alpha})$$
$$-6!\frac{\hbar^2}{2M}\frac{n(n+1)-L(L+1)}{1.33N^2}\int(\psi_0-2\psi_1+\psi_2)^*$$
$$\times\frac{1}{R^2}\psi_0 d\tau-6!\frac{\hbar^2}{2M}\frac{1}{N^2}\int(\psi_0-2\psi_1+\psi_2)^*$$
$$\times(\alpha^2\sum_{i=1}^{4}\rho_i^2+\bar{\alpha}^2\sum_{j=5}^{6}\rho_j^2+\tfrac{4}{3}\beta^2R^2)\psi_0 d\tau, \quad (11)$$

$$\langle V\rangle=\langle V_c\rangle+\langle V_{so}\rangle$$
$$=(6!/N^2)\left\{\int\psi_0^*[w(12F_{12}+6F_{15}+2F_{56})\right.$$
$$+\epsilon_1 b(2F_{56})]\psi_0 d\tau$$
$$-\int\psi_1^*[w(-6F_{15}+12F_{23}+8F_{16}+24F_{12}+2F_{26})$$
$$+\epsilon_1 b(8F_{16}-4F_{26})]\psi_0 d\tau$$
$$+\int\psi_2^*[w(4F_{12}+16F_{13}-2F_{15}+2F_{34})$$
$$\left.+\epsilon_1 b(4F_{12}-8F_{13}+4F_{15}+2F_{34})]\psi_0 d\tau\right\}$$
$$+(6!/N^2)\epsilon_2\left\{\int\psi_0^*(4G_{15})\psi_0 d\tau\right.$$
$$-2\int\psi_1^*(G_{15}+G_{25}+G_{16}+G_{26})\psi_0 d\tau$$
$$\left.+\int\psi_2^*(4G_{15})\psi_0 d\tau\right\}, \quad (12)$$

where

$$F_{ij}=-V_0\exp(-\kappa r_{ij}^2), \quad (13)$$

and

$$G_{ij}=-V_{LS}\exp(-\lambda r_{ij}^2)[\hbar^{-1}(\mathbf{r}_i-\mathbf{r}_j)\times(\mathbf{p}_i-\mathbf{p}_j)]_z, \quad (14)$$

with the subscript z denoting the z component of the expression within the bracket. Also, in Eq. (12), ϵ_1 is equal to 1 for triplet states and -1 for singlet states,

[26] F. Ajzenberg-Selove and T. Lauritsen, "Energy levels of light nuclei ($A=5$ to 20)," Tech. Rept. (1960).
[27] S. F. Edwards, Proc. Cambridge Phil. Soc. 48, 652 (1952).

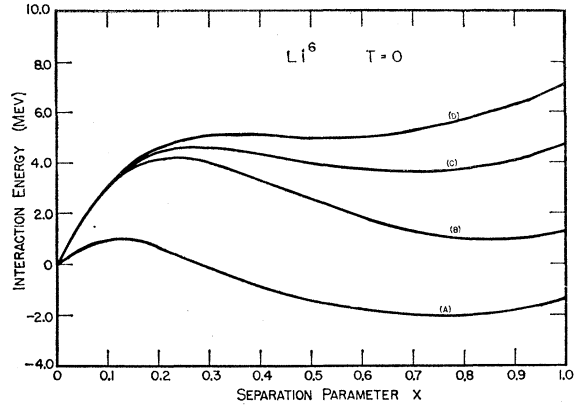

FIG. 1. $T=0$ states of Li^6 with y and z at their optimizing values: (A) $^3S_1$, (B) $^3D_3$, (C) $^3D_2$, (D) $^3D_1$.

and ϵ_2 has the value 1, $-\frac{1}{2}$, $-\frac{3}{2}$ for the states $^3D_3$, $^3D_2$, $^3D_1$, respectively, and zero for all other states considered in this investigation. Coulomb energy has not been included in Eq. (12); it will be computed in an approximate manner and discussed in a later paragraph.

The internal energy of the deuteron cluster is calculated with the Serber force given by Eq. (3), while for the energy of the alpha cluster, we adopt the expression

$$E_\alpha = -28.3 + 33.4(1-0.96/y)^2 \text{ Mev}, \quad (15)$$

where for computational purposes, we have redefined the variational parameters as

$$x=\beta/\alpha, \quad y=\kappa/\alpha, \quad z=\bar{\alpha}/\alpha. \quad (16)$$

The constants in Eq. (15) are so chosen that the alpha particle binding energy and rms radius are given correctly. Also, the compressibility implied by Eq. (15) is consistent with the nuclear compressibility determined from analyses of the isotope shifts.[28]

Since the Coulomb interaction is a long-range operator, we shall calculate the interaction Coulomb energy between two clusters with an unantisymmetrized wave function, i.e.,

$$E_{\text{Coul}}=\left[2e^2\int\psi_0^*(1/R)\psi_0 d\tau\right]\Big/\left[\int\psi_0^*\psi_0 d\tau\right]. \quad (17)$$

A check with an exact calculation for one particular set of parameters indicates that Eq. (17) overestimates the interaction Coulomb energy by about 10%.

With Eqs. (9), (11), and (12), we are led to an expression for the expectation value of the Hamiltonian in terms of the variational parameters x, y, and z. To obtain the interaction energy between the clusters, we must further subtract off from the aforementioned expression the internal energies calculated with the Serber force and add to it the interaction Coulomb energy. Finally, by adding the deuteron cluster internal energy E_d and the alpha cluster internal energy E_α, we obtain the energy of the state in question, which must now be minimized with respect to all the variational parameters.

TABLE I. Calculated energies for the first six levels in Li^6.

	Terms	X	Y	Z	Calculated energies (Mev)
$T=0$	$^3S_1$	0.76	0.96	1.52	−30.0
	$^3D_3$	0.86	0.96	1.51	−27.0
	$^3D_2$	0.71	0.96	1.33	−24.7
	$^3D_1$	0.52	0.96	1.16	−23.5
$T=1$	$^1S_0$	0.75	0.96	0.98	−24.4
	$^1D_2$	0.68	0.96	0.80	−21.7

The complete numerical analysis was performed on an IBM 650 computer. The interaction energy of each state as a function of the parameter x with y and z at their optimizing values is plotted in Figs. 1 and 2 (Fig. 1 for $T=0$ states and Fig. 2 for $T=1$ states). For the range parameter λ of the spin-orbit potential, we have chosen the value 2.657×10^{25} cm^{-2} used by Hochberg *et al.*[29] in their analysis on the scattering of nucleons by alpha particles. The depth V_{LS} is then adjusted to yield the correct $^3D_3-^3D_2$ splitting. With this procedure, V_{LS} is found to be equal to 1.90 Mev, comparing to the value of 4.5 Mev attained by Hochberg *et al.* Shorter ranges with λ equal to 4.16×10^{25} cm^{-2} and 5.663×10^{25} cm^{-2} have also been tried, the corresponding depths then turn out to be 3.91 and 7.08 Mev, respectively.

The results for the total energies of the various states and the optimizing values for the variational parameters are listed in Table I. In this table, the values listed are obtained with the parameters λ and V_{LS} of the spin-orbit potential having the values 2.657×10^{25} cm^{-2} and 1.90 Mev, respectively. For other choices of the latter parameters, the results are slightly different; the difference is, however, so small that it is not worthy of listing.

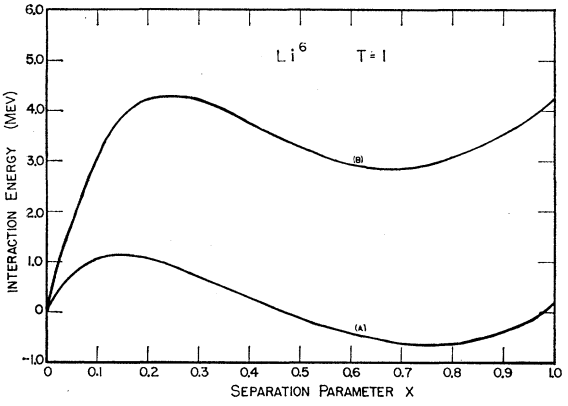

FIG. 2. $T=1$ states of Li^6 with y and z at their optimizing values: (A) $^1S_0$, (B) $^1D_2$.

[28] D. L. Hill, *Encyclopedia of Physics*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 39, p. 203.

[29] S. Hochberg, H. S. W. Massey, H. Robertson, and L. H. Underhill, Proc. Phys. Soc. (London) **A68**, 746 (1955).

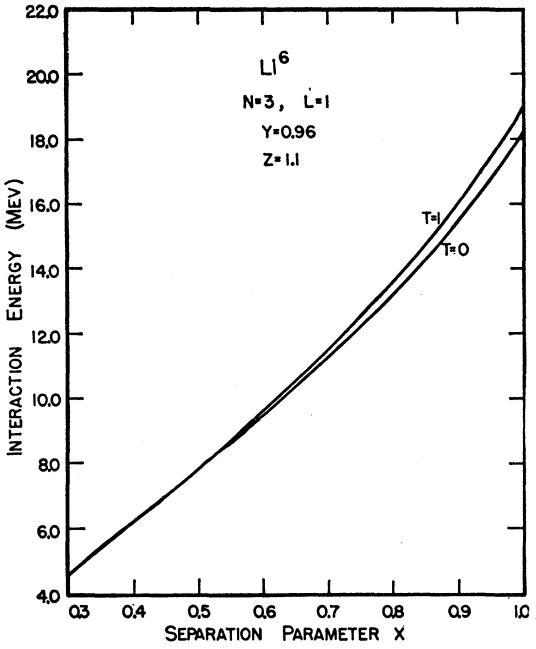

FIG. 3. Interaction energy as a function of the separation parameter for the alpha-deuteron configuration with $n=3$, $L=1$.

Using the cluster wave function (5) and the values of the variational parameters in Table I, we have also computed the rms radius of Li^6 in the ground state from the expression

$$R_{\rm rms}=\left\{\left(\frac{6!}{N^2}\right)\int(\psi_0-2\psi_1+\psi_2)^* \times\left[\tfrac{1}{6}\left(\sum_{i=1}^{6}\rho_i^2+\tfrac{4}{3}R^2\right)\right]\psi_0 d\tau\right\}^{\frac{1}{2}}, \quad (18)$$

and obtained 2.02 fermi as compared with the 2.70 fermi found by the electron scattering experiment.[30]

To corroborate our contention that the configuration of an alpha cluster in relative $3p$-state motion ($n=3$, $L=1$) with an s-state deuteron cluster cannot properly describe a resonant state, we have performed the desired calculation including the two-body central potential only and determined the interaction energy as a function of the separation parameter x, which is plotted in Fig. 3. We note that these curves possess absolutely no trace of a relative minimum, indicating the absence of resonant states with such configurations.

IV. ENERGY LEVELS OF Li^7 AND Be^7

A. Qualitative Description

To describe the states with the highest space symmetry in Li^7, it is most convenient to use an alpha cluster plus a triton cluster representation. In the first approximation, these states can then be described by a pure cluster configuration in which neither the alpha cluster nor the triton cluster is excited. Since, in the single-particle shell model picture, three nucleons are in the 1 p-shell, the relative motion between the clusters must be an oscillation of third order with $L=1$ or 3 to comply with the Pauli exclusion principle. The $L=1$ configuration gives rise to the ^2P doublets, while the $L=3$ configuration yields the ^2F states. This predicted structure is in agreement with the experimentally determined level scheme.

Again, the adoption of the $L-S$ coupling scheme finds support from the results of the intermediate-coupling calculation.[10] For Li^7, the rather small value of the intermediate coupling parameter indicates that the coupling is near the $L-S$ limit.

From a study of the excitation energies of the mirror levels in Li^7 and Be^7,[18] we can conclude that the $(\frac{5}{2}-)$ level at 7.47 Mev in Li^7 (7.18 Mev in Be^7) must essentially have a different structure from that of the ^2P and ^2F doublets.[31] Thus, for its description, it is more convenient to choose a Li^6 cluster plus a neutron representation,[32] since, in this representation, this state can be described in first approximation by a pure configuration, i.e., an unexcited Li^6 cluster and a neutron in relative $1p$-state ($n=1$, $L=1$) motion. With such a description, this state is then a member of the ^4P multiplet, in agreement with the predictions of many other authors.[6–8]

The existence of a broad positive-parity level around 6.6 Mev in Li^7 [5,33] is rather difficult to explain in our picture. In the Li^6 cluster-plus-neutron representation, this state would mainly be described by a relative $2s$ ($n=2$, $L=0$) motion between the clusters; thus, energetically, it is expected to lie above the $(\frac{5}{2}-)$ level at 7.47 Mev.[34] In fact, from our experience of cluster model calculations, we would even suspect whether this configuration could properly describe a resonant state. Recent failure in finding this level experimentally by the (d,p) reaction on Li^6 [35] also seems to indicate that the presence of this level may be seriously in question. Theoretical computations are now being undertaken to prove or disprove its existence.

B. Quantitative Treatment

As we shall only calculate the energies of the ^2P and ^2F doublets, we choose the trial wave function in the

[30] R. Hofstadter, Revs. Modern Phys. 28, 214 (1956); G. R. Burleson and R. Hofstadter, Phys. Rev. 112, 1282 (1958); N. Meyer-Berkhout, K. W. Ford, and A. E. S. Green, Ann. Phys. (N. Y.) 8, 119 (1959).

[31] This conclusion can also be reached by studying the various reduced partial widths of this level.

[32] This is equivalent to an alpha cluster plus deuteron cluster plus nucleon representation.

[33] C. A. Levinson and M. K. Banerjee, Ann. Phys. 2, 471 (1957).

[34] This corrects a mistaken statement in I wherein we asserted that this state lies lower than the $(\frac{5}{2}-)$ level at 7.47 Mev.

[35] E. W. Hamburger and J. R. Cameron, Phys. Rev. 117, 781 (1960).

form

$$\Psi=A\{\psi(1234;567)\xi(1234;567)\}$$
$$=A\left\{\exp\left(-\frac{\alpha}{2}\sum_{i=1}^{4}\rho_i^2\right)\exp\left(-\frac{\bar{\alpha}}{2}\sum_{j=5}^{7}\rho_j^2\right)\right.$$
$$\left.\times R^n Y_{LM}(\mathbf{R}/R)\exp\left(-\frac{6}{7}\beta R^2\right)\xi(1234;567)\right\}, \quad (19)$$

which again reduces to the usual shell model wave function describing the lowest configuration $(1s)^4(1p)^3$ in an oscillator well of width parameter α, if β and $\bar{\alpha}$ are set equal to α. Also in Eq. (19), all quantities have analogous meanings to the corresponding ones in Sec. III B; hence, they will not be further explained.

The quantity n will assume the value 3 as explained in Sec. IV A, while the orbital angular momentum quantum number L will take on the values 1 and 3 for the ^2P doublet and the ^2F doublet, respectively.

With the wave function (19) and the two-body force (3), the normalization factor N^2, kinetic energy $\langle T\rangle$ and potential energy $\langle V\rangle$ can again be easily calculated. They have the following forms[36]:

$$N^2=7!\int(\psi_0-3\psi_1+3\psi_2-\psi_3)^*\psi_0 d\tau, \quad (20)$$

where

$$\psi_0=\psi(1234;567),\quad \psi_2=\psi(5634;127),$$
$$\psi_1=\psi(5234;167),\quad \psi_3=\psi(5674;123), \quad (21)$$

with the subscripts 0, 1, 2, 3 denoting no-exchange, one-exchange, two-exchange, and three-exchange, respectively.

$$\langle T\rangle=\frac{\hbar^2}{2M}(2n\beta+3\beta+9\alpha+6\bar{\alpha})$$
$$-7!\frac{\hbar^2}{2M}\frac{n(n+1)-L(L+1)}{12N^2/7}\int(\psi_0-3\psi_1+3\psi_2-\psi_3)^*$$
$$\times\frac{1}{R^2}\psi_0 d\tau-7!\frac{\hbar^2}{2M}\frac{1}{N^2}\int(\psi_0-3\psi_1+3\psi_2-\psi_3)^*$$
$$\times\left(\alpha^2\sum_{i=1}^{4}\rho_i^2+\bar{\alpha}^2\sum_{j=5}^{7}\rho_j^2+\frac{12}{7}\beta^2R^2\right)\psi_0 d\tau. \quad (22)$$

$$\langle V\rangle=\langle V_c\rangle+\langle V_{so}\rangle$$
$$=(7!/N^2)\left\{\int\psi_0^*[w(12F_{12}+9F_{15}+6F_{56})]\psi_0 d\tau\right.$$
$$-\int\psi_1^*[w(-9F_{15}+18F_{23}+24F_{16}$$
$$+36F_{12}+6F_{26}+6F_{67})]\psi_0 d\tau$$
$$+\int\psi_2^*[w(-6F_{15}+12F_{12}+24F_{17}$$
$$-3F_{37}+48F_{13}+6F_{34})]\psi_0 d\tau$$
$$\left.-\int\psi_3^*[w(3F_{15}+12F_{12}+12F_{14})]\psi_0 d\tau\right\}$$
$$+(7!/N^2)\epsilon_2\int\left\{\psi_0^*(2G_{15})\psi_0 d\tau\right.$$
$$-\int\psi_1^*(G_{15}+2G_{16}+G_{25}+2G_{26})\psi_0 d\tau$$
$$+\int\psi_2^*(4G_{15}+2G_{17})\psi_0 d\tau$$
$$\left.-\int\psi_3^*(3G_{15}-G_{45})\psi_0 d\tau\right\}, \quad (23)$$

in which F_{ij} and G_{ij} are defined by Eqs. (13) and (14). Also, ϵ_2 is equal to 1, -2, 1 and $-\frac{4}{3}$ for the $^2P_{\frac{3}{2}}$, $^2P_{\frac{1}{2}}$, $^2F_{7/2}$ and $^2F_{\frac{5}{2}}$ states, respectively.

The internal energy of the alpha cluster is given by Eq. (15), while that of the triton cluster is represented by the expression

$$E_T=-8.5+8.6(1-1.41/y)^2 \text{ Mev}, \quad (24)$$

where, again, the constants are so chosen that the triton binding energy and rms radius are given correctly.[37]

The complete numerical analyses can now be performed with exactly the same procedure as outlined in Sec. III B. The interaction energy of each of the four states as a function of the parameter x with y and z at their optimizing values is plotted in Fig. 4. With the range parameter λ of the spin-orbit potential set equal to 2.657×10^{25} cm^{-2}, it is found that a depth V_{LS} of 1.66 Mev will produce the proper ^2P splitting. This value of V_{LS} is somewhat smaller than that needed to account

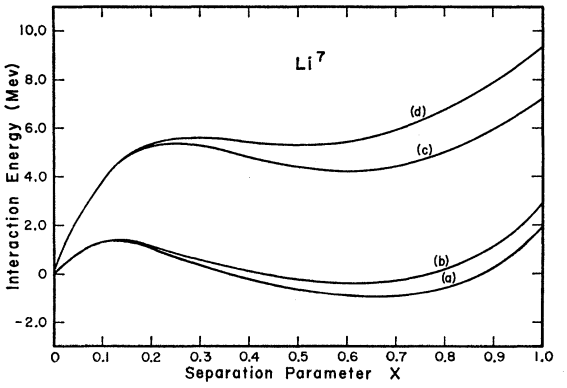

FIG. 4. Energy levels of Li^7 with y and z at their optimizing values: (a) $^2P_{\frac{1}{2}}$, (b) $^2P_{\frac{3}{2}}$, (c) $^2F_{7/2}$, (d) $^2F_{\frac{5}{2}}$.

[36] The potential integrals for the limiting case of $z=1$ have already been given in I; hence, they will not be listed in the Appendix.

[37] B. C. Carlson and I. Talmi, Phys. Rev. **96**, 436 (1954).

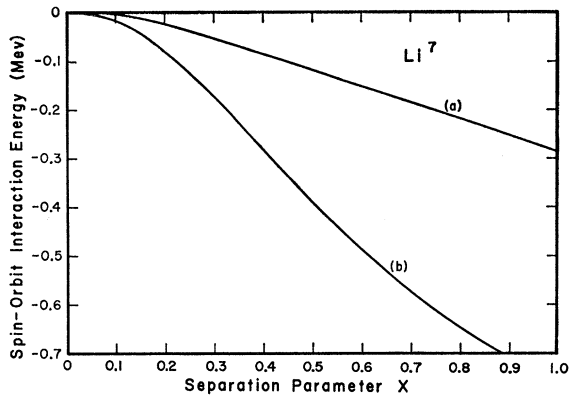

FIG. 5. Spin-orbit interaction energy in Li^7 as a function of the separation parameter with y and z at their optimizing values: (a) $^2P_{\frac{3}{2}}$, (b) $^2F_{7/2}$.

for the splittings in Li^6. Other ranges at λ equal to 4.16×10^{25} cm^{-2} and 5.663×10^{25} cm^{-2} have also been tried, the corresponding depths are then calculated to be 3.78 and 7.03 Mev, respectively, again smaller than the corresponding values in Li^6.

The behavior of the interaction spin-orbit energy as a function of x for the state $^2P_{\frac{3}{2}}$ and the state $^2F_{7/2}$ is plotted in the graphs of Fig. 5. For these curves, λ and V_{LS} are set as 2.657×10^{25} cm^{-2} and 1.66 Mev, respectively.

The results for the total energies of the various states in Li^7 and the optimizing values for the variational parameters are listed in Table II. In Table III, we list the excitation energies of the $^2P_{\frac{1}{2}}$, $^2F_{7/2}$ and $^2F_{\frac{5}{2}}$ levels in both Li^7 and Be^7. We note that the calculated $(\frac{5}{2}-)$ level occurs at an excitation of 5.96 Mev in Li^7 and 5.85 Mev in Be^7. Taking into account the fact that our variational wave function overestimates the excitation of the $^2F_{7/2}$ level by about 0.3 Mev, we venture to say that the actual locations of the $(\frac{5}{2}-)$ levels are at about 5.6 Mev in Li^7 and 5.5 Mev in Be^7.

To discuss the property of the $^2F_{\frac{5}{2}}$ level, we note that in Fig. 4, curve (d), which exhibits the behavior of the interaction energy of this level, has a very shallow relative minimum, which is a consequence of the fact that in this state, the spin-orbit interaction is relatively strong and repulsive. By studying the correlation between the depths of the relative minima and the known level widths of many other levels considered in our cluster model calculations, we can conclude, although

TABLE II. Energy levels of Li^7.[a]

Terms	X	Y	Z	Calculated energies (Mev)
$^2P_{3/2}$	0.65	0.96	0.80	−37.4
$^2P_{1/2}$	0.61	0.96	0.79	−36.9
$^2F_{7/2}$	0.59	0.97	0.74	−32.5
$^2F_{5/2}$	0.52	0.98	0.70	−31.5

[a] Computed with $\lambda=2.657\times10^{25}$ cm^{-2} and $V_{LS}=1.66$ Mev.

TABLE III. Excitation energies of levels in Li^7 and Be^7.[a]

Terms	Excitation energies in Li^7 (Mev) Calculated	Excitation energies in Li^7 (Mev) Experimental	Excitation energies in Be^7 (Mev) Calculated	Excitation energies in Be^7 (Mev) Experimental
$^2P_{3/2}$	0	0	0	0
$^2P_{1/2}$	0.48	0.478	0.44	0.431
$^2F_{7/2}$	4.94	4.63	4.89	4.54
$^2F_{5/2}$	5.96		5.85	

[a] Computed with $\lambda=2.657\times10^{25}$ cm^{-2} and $V_{LS}=1.66$ Mev.

only in a qualitative manner, that the level width of this $(\frac{5}{2}-)$ state must be quite large, perhaps in the neighborhood of 1 Mev or so. This large level width, together with the fact that there are other levels of similar widths around, makes the experimental determination of this level rather difficult.[38,39] The most promising way to explore this level experimentally seems to be by $H^3(He^3)-He^4$ scattering; this is so, since this level is energetically incapable of decaying into Li^6 plus a nucleon, and reactions such as (d,p) on Li^6 are not suitable for the study of ^2F levels.

Finally, we have also computed the rms radius of the ground state of Li^7 from an expression similar to Eq. (18). We obtain a value 2.28 fermi as compared to 2.71 fermi found by the electron scattering experiment.[30]

V. SUMMARY AND DISCUSSION

In this section we present an analysis of all our cluster model calculations performed to date. The complete final results along with the appropriate experimental values are tabulated in Table IV.

TABLE IV. Summary of results.[a]

Nucleus	T	J^π	E_{calc} (Mev)	E_{exp} (Mev)	$E_{\text{calc}}-E_{\text{exp}}$ (Mev)
He^5	$\frac{1}{2}$	$\frac{3}{2}-$	−25.4	−27.3	1.9
		$\frac{3}{2}+$	−8.3	−10.6	2.3
Li^6	0	1+	−30.0	−32.0	2.0
		3+	−27.0	−29.8	2.8
		2+	−24.7	−27.5	2.8
		1+	−23.5	−26.5	3.0
	1	0+	−24.4	−28.4	4.0
		2+	−21.7	−26.6	4.9
Li^7	$\frac{1}{2}$	$\frac{3}{2}-$	−37.4	−39.2	1.8
		$\frac{1}{2}-$	−36.9	−38.7	1.8
		$\frac{7}{2}-$	−32.5	−34.6	2.1
		$\frac{5}{2}-$	−31.5		
Be^8	0	0+	−57.1	−56.5	−0.6
		2+	−53.8	−53.6	−0.2
		4+	−45.5	−45.2	−0.3

[a] All experimental values are taken from reference 26.

[38] See also remarks by Marion, reference 8.

[39] Morinaga (reference 4, p. 418) recently reported that he has seen a broad $L=3$ resonance from He^3+He^4 scattering in the energy range from 13 to 19 Mev. Since the energy range in his experiment corresponds to an excitation energy in Be^7 of about 9 to 12 Mev, we do not believe that the $L=3$ state which he found is the $(\frac{5}{2}-)$ level we are concerned with.

Of primary importance is the question of convergence; that is to say, are our results markedly changed by the inclusion of additional variational parameters? The present Li^7 calculation, which is performed with an additional variational parameter, produces only a minor change in the energies of the ^2P and ^2F doublets, namely, 0.4 and 0.7 Mev, respectively. We are thus encouraged to believe that our method does converge fairly rapidly. It should be remarked at this point that for reasonable results there must be a minimum number of variational parameters in the trial wave function; the exact number is determined from the cluster structure of the level, as described in Secs. III and IV.

In actuality, those wave functions which consist in part of a deuteron substructure do not contain an adequate number of parameters. This can best be seen by examining the internal energy and rms radius of the deuteron. The simple Gaussian function which describes this cluster cannot possibly produce the appropriate properties of a free deuteron. In fact, it is found that the binding energy so calculated is 0.27 Mev and the rms radius is only 1.25 fermi. However, a wave function which is comprised of the sum of two Gaussians allows for values which are considerably better. This latter shortcoming leads to discrepancies in the energies of the levels of Li^6 and the $(\frac{3}{2}+)$ state of He^5. This is especially apparent for the $T=1$ states of Li^6 wherein the energies are overestimated by as much as 4 Mev; this discrepancy can be easily understood by noting that for the $T=1$ states, the deuteron itself is in an unbound singlet state which implies that a single Gaussian wave function is even less appropriate.

A probable source of error in our calculation arises from the relatively simple choice for the two-body potential. However, since our intention is to survey the energies of the lower-lying levels of the light nuclei, any minor change in our final results is uninteresting. In fact, it is found that reasonable modifications of the two-body potential produces changes in the final results which, in the spirit of the above remark, are of little concern.

One question which still remains to be answered is concerned with the actual form of the two-body spin-orbit force. Unfortunately, there is at present no such potential which can be inferred from low-energy nucleon-nucleon phenomena. Hence, we must resort to a less palatable method of obtaining the spin-orbit force, namely, an analysis of the structure of the light nuclei.

TABLE V. Depth of spin-orbit potential.

λ (10^{-25} cm^{-2})	V_{LS} (Mev) He^5	Li^6	Li^7
2.657	4.5[a]	1.90	1.66
4.16	9.86	3.91	3.78
5.663	17.88	7.08	7.03

[a] Taken from Hochberg *et al.*, reference 29.

The results of a computation using a simple neutral form for the nuclei He^5, Li^6, and Li^7 are tabulated in Table V. For each choice of range λ, we have found the depth V_{LS} which produces the experimental splittings. We note immediately that the He^5 results are totally inconsistent with the other values. Moreover, the agreement between the Li^6 and Li^7 values is considered to be coincidental since the tabulated depths for Li^6 would be increased by about 25% had we used a better trial function for the deuteron cluster. It is thus our contention that the spin-orbit potential is not of the neutral form alone, but includes an isotopic spin dependent component. The confirmation of this latter assertion awaits a more detailed calculation; one in which the deuteron cluster is treated as previously proposed.

Upon concluding this phase of our investigation of the behavior of light nuclei with $A=5$, 6, 7, 8, we would like to briefly discuss the possibility of extending our method of calculation to heavier nuclei. For reasons of simplicity, we have always assumed a pure configuration for the cluster wave functions. As has been discussed in Secs. III and IV, this is probably a good approximation for the above-mentioned nuclei. On the other hand, there is strong evidence that already for B^{10}, the spin-orbit interaction becomes so strong that the $L-S$ coupling scheme ceases to hold.[10] Thus, to extend our calculation to heavier nuclei, we must relinquish the assumption of pure configurations and describe all nuclear states by a mixture of different cluster wave functions.

In addition, as has been mentioned in I and II, one must devise a way to include the hard-core part of the nuclear force more consistently. The approximations involved in our method of calculation as described in Sec. II are necessitated by the fact that with a Serber force of the form (3), the binding energies and rms radii of a free alpha particle and of a triton cannot be reproduced. One obvious method of improvement is to use a simple two-body force with a repulsive core (not infinitely hard) which can account for the bound state data of two-, three- and four-body systems and at the same time, explain the scattering data of *p-p* and *n-p* systems up to about 50 Mev. Further, one must introduce in the trial wave function a short-range correlation factor of the form

$$\prod_{\text{all pairs}} [1-\exp(-\gamma r_{ij}^2)] \tag{25}$$

to reduce the probability that two nucleons get within the range of the repulsive core. This particular correlation factor is preferred since it does not disturb the geometrical properties of the simpler cluster functions, namely, L and S are still good quantum numbers and further, spurious states due to improper treatment of the center-of-mass motion do not arise. Initial effort with such a procedure is now being undertaken to calculate the energies of the levels of Be^8. Satisfactory results will not only encourage us to investigate heavier

nuclei, but also will strengthen our present belief that results so far obtained with the simpler method are likely reliable.

APPENDIX

Potential Integrals of Li^6

The method of evaluating the expectation values of the various operators has been discussed in I and in the Appendix of II; hence, only the results will be presented here.

The normalization factor is given by the expression

$$N^2=6![A_0-2A_1+A_2], \tag{A.1}$$

with

$$A_0=2^9\left(\frac{\pi^3}{4\alpha^3}\right)^{\frac{3}{2}}\left(\frac{\pi}{2\bar{\alpha}}\right)^{\frac{3}{2}}I_{2n+2,l}(\beta),$$

$$A_1=\Gamma\left[\frac{\pi^2}{\alpha(4\alpha+6\bar{\alpha})}\right]^{\frac{3}{2}}J_{n+2,n+2,l}\left(\frac{\omega}{\sigma}+\beta,-\frac{\xi}{\sigma},\frac{\omega}{\sigma}+\beta\right), \tag{A.2}$$

$$A_2=\Gamma(\tfrac{1}{2})^3\left(\frac{\pi}{\alpha+\bar{\alpha}}\right)^3J_{n+2,n+2,l}\left(\frac{5}{3}\alpha+\beta,\frac{8}{3}\alpha,\frac{5}{3}\alpha+\beta\right),$$

where

$$\begin{aligned}\Gamma&=2^9(\tfrac{4}{3})^3(\pi/\alpha)^{\frac{3}{2}},\\ \sigma&=6\alpha+9\bar{\alpha},\\ \omega&=3\alpha^2+11\alpha\bar{\alpha}+3\bar{\alpha}^2,\\ \xi&=6\alpha^2+4\alpha\bar{\alpha}+6\bar{\alpha}^2,\end{aligned} \tag{A.3}$$

and

$$I_{\mu l}(p)=\int R^\mu\exp(-\tfrac{4}{3}pR^2)\,|\,Y_{lm}(\mathbf{R}/R)\,|^2dRd\Omega, \tag{A.4}$$

$$J_{\mu\nu l}(p,q,s)=\int R'^\mu R^\nu\exp[-\tfrac{2}{3}(pR'^2+q\mathbf{R}'\cdot\mathbf{R}+sR^2)]\times Y_{lm}(\mathbf{R}'/R')Y_{lm}^*(\mathbf{R}/R)dR'dRd\Omega'd\Omega. \tag{A.5}$$

For the various terms of the potential energy, we have [see Eq. (12)]:

$$F_{12}^0=-V_0\left\{\left(\frac{\alpha}{\alpha+2\kappa}\right)^{\frac{3}{2}}A_0\right\}, \tag{A.6}$$

$$F_{15}^0=-V_0\left\{2^9\left(\frac{\pi}{\alpha}\right)^3\left[\frac{\pi^2}{8\alpha\bar{\alpha}+\kappa(4\alpha+6\bar{\alpha})}\right]^{\frac{3}{2}}I_{2n+2,l}\left(\beta+\frac{6\alpha\bar{\alpha}\kappa}{8\alpha\bar{\alpha}+\kappa(4\alpha+6\bar{\alpha})}\right)\right\}, \tag{A.7}$$

$$F_{56}^0=-V_0\left\{\left(\frac{\bar{\alpha}}{\bar{\alpha}+2\kappa}\right)^{\frac{3}{2}}A_0\right\}, \tag{A.8}$$

$$F_{15}^1=-V_0\left\{\Gamma\left[\frac{\pi^2}{\alpha(4\alpha+6\bar{\alpha})}\right]^{\frac{3}{2}}J_{n+2,n+2,l}\left(\frac{\omega}{\sigma}+\beta+\frac{8}{3}\kappa,-\frac{\xi}{\sigma}-\frac{16}{3}\kappa,\frac{\omega}{\sigma}+\beta+\frac{8}{3}\kappa\right)\right\}, \tag{A.9}$$

$$F_{23}^1=-V_0\left\{\left(\frac{\alpha}{\alpha+2\kappa}\right)^{\frac{3}{2}}A_1\right\}, \tag{A.10}$$

$$F_{16}^1=-V_0\left\{\Gamma\left[\frac{\pi^2}{\alpha(4\alpha+6\bar{\alpha}+12\kappa)}\right]^{\frac{3}{2}}J_{n+2,n+2,l}\left(\frac{\omega+34\alpha\kappa+12\bar{\alpha}\kappa}{\sigma+18\kappa}+\beta,-\frac{\xi+8\alpha\kappa+24\bar{\alpha}\kappa}{\sigma+18\kappa},\frac{\omega+10\alpha\kappa+12\bar{\alpha}\kappa}{\sigma+18\kappa}+\beta\right)\right\}, \tag{A.11}$$

$$F_{12}^1=-V_0\left\{\Gamma\left[\frac{\pi^2}{4\alpha^2+6\alpha\bar{\alpha}+4\kappa(2\alpha+\bar{\alpha})}\right]^{\frac{3}{2}}J_{n+2,n+2,l}\left[\frac{\alpha\omega+\kappa(10\alpha^2+10\alpha\bar{\alpha}+2\bar{\alpha}^2)}{\alpha\sigma+6\kappa(2\alpha+\bar{\alpha})}+\beta,-\frac{\alpha\xi+\kappa(20\alpha^2+8\alpha\bar{\alpha}+4\bar{\alpha}^2)}{\alpha\sigma+6\kappa(2\alpha+\bar{\alpha})},\frac{\alpha\omega+\kappa(10\alpha^2+34\alpha\bar{\alpha}+2\bar{\alpha}^2)}{\alpha\sigma+6\kappa(2\alpha+\bar{\alpha})}+\beta\right]\right\}, \tag{A.12}$$

$$F_{26}^1=-V_0\left\{\Gamma\left[\frac{\pi^2}{4\alpha^2+6\alpha\bar{\alpha}+4\kappa(\alpha+\bar{\alpha})}\right]^{\frac{3}{2}}J_{n+2,n+2,l}\left[\frac{\alpha\omega+2\kappa(\alpha+\bar{\alpha})(6\alpha+\bar{\alpha})}{\alpha\sigma+6\kappa(\alpha+\bar{\alpha})}+\beta,-\frac{\alpha\xi-2\kappa(\alpha+\bar{\alpha})(6\alpha-2\bar{\alpha})}{\alpha\sigma+6\kappa(\alpha+\bar{\alpha})},\frac{\alpha\omega+2\kappa(\alpha+\bar{\alpha})(6\alpha+\bar{\alpha})}{\alpha\sigma+6\kappa(\alpha+\bar{\alpha})}+\beta\right]\right\}, \tag{A.13}$$

$$F_{12}^2=-V_0\left\{\left(\frac{\alpha+\bar{\alpha}}{\alpha+\bar{\alpha}+4\kappa}\right)^{\frac{3}{2}}A_2\right\}, \tag{A.14}$$

$$F_{13}^{2}=-V_0\left\{\Gamma\left(\frac{\alpha}{\alpha+\bar{\alpha}}\right)^{\frac{3}{2}}\left[\frac{\pi^2}{2\alpha^2+2\alpha\bar{\alpha}+\kappa(3\alpha+\bar{\alpha})}\right]^{\frac{3}{2}}J_{n+2,n+2,l}\left[\frac{10\alpha^2(\alpha+\bar{\alpha})+\alpha\kappa(19\alpha+9\bar{\alpha})}{6\alpha(\alpha+\bar{\alpha})+3\kappa(3\alpha+\bar{\alpha})}+\beta,\right.\right.$$
$$\left.\left.\frac{16\alpha^2(\alpha+\bar{\alpha})+8\alpha\kappa(5\alpha+3\bar{\alpha})}{6\alpha(\alpha+\bar{\alpha})+3\kappa(3\alpha+\bar{\alpha})},\frac{10\alpha^2(\alpha+\bar{\alpha})+\alpha\kappa(31\alpha+21\bar{\alpha})}{6\alpha(\alpha+\bar{\alpha})+3\kappa(3\alpha+\bar{\alpha})}+\beta\right]\right\},\quad\text{(A.15)}$$

$$F_{15}^{2}=-V_0\left\{\Gamma\left[\frac{\pi^2}{(\alpha+\bar{\alpha})(2\alpha+2\bar{\alpha}+4\kappa)}\right]^{\frac{3}{2}}J_{n+2,n+2,l}\left[\frac{5\alpha(\alpha+\bar{\alpha})+2\kappa(6\alpha+\bar{\alpha})}{3\alpha+3\bar{\alpha}+6\kappa}+\beta,\right.\right.$$
$$\left.\left.\frac{8\alpha(\alpha+\bar{\alpha})+\kappa(12\alpha-4\bar{\alpha})}{3\alpha+3\bar{\alpha}+6\kappa},\frac{5\alpha(\alpha+\bar{\alpha})+2\kappa(6\alpha+\bar{\alpha})}{3\alpha+3\bar{\alpha}+6\kappa}+\beta\right]\right\},\quad\text{(A.16)}$$

$$F_{34}^{2}=-V_0\left\{\left(\frac{\alpha}{\alpha+2\kappa}\right)^{\frac{3}{2}}A_2\right\},\quad\text{(A.17)}$$

and

$$G_{15}^{0}=-V_{LS}\left\{2^9\left(\frac{\pi}{\alpha}\right)^3\left[\frac{\pi^2}{8\alpha\bar{\alpha}+\lambda(4\alpha+6\bar{\alpha})}\right]^{\frac{3}{2}}\left[\frac{6\alpha\bar{\alpha}}{4\alpha\bar{\alpha}+\lambda(2\alpha+3\bar{\alpha})}\right]I_{62}\left[\beta+\frac{6\alpha\bar{\alpha}\lambda}{8\alpha\bar{\alpha}+\lambda(4\alpha+6\bar{\alpha})}\right]\right\},\quad\text{(A.18)}$$

$$G_{15}^{1}=-V_{LS}\left\{\Gamma\left[\frac{\pi^2}{\alpha(4\alpha+6\bar{\alpha})}\right]^{\frac{3}{2}}\left[2J_{442}\left(\frac{\omega}{\sigma}+\beta+\frac{8}{3}\lambda,-\frac{\xi}{\sigma}-\frac{16}{3}\lambda,\frac{\omega}{\sigma}+\beta+\frac{8}{3}\lambda\right)\right.\right.$$
$$\left.\left.-2J_{351}+\frac{40\alpha\bar{\alpha}-16\alpha\beta-24\bar{\alpha}\beta}{5\sigma}(J_{553}-J_{551})\right]\right\},\quad\text{(A.19)}$$

$$G_{25}^{1}=-V_{LS}\left(\Gamma\left(\frac{3\pi^2}{2}\right)^{\frac{3}{2}}\left[\frac{1}{\alpha\sigma+6\lambda(2\alpha+\bar{\alpha})}\right]^{\frac{5}{2}}\left\{(6\alpha^2+18\alpha\bar{\alpha})J_{442}\left[\frac{\alpha\omega+\lambda(10\alpha^2+34\alpha\bar{\alpha}+2\bar{\alpha}^2)}{\alpha\sigma+6\lambda(2\alpha+\bar{\alpha})}+\beta,\right.\right.\right.$$
$$\left.\left.\left.-\frac{\alpha\xi+\lambda(20\alpha^2+8\alpha\bar{\alpha}+4\bar{\alpha}^2)}{\alpha\sigma+6\lambda(2\alpha+\bar{\alpha})},\frac{\alpha\omega+\lambda(10\alpha^2+10\alpha\bar{\alpha}+2\bar{\alpha}^2)}{\alpha\sigma+6\lambda(2\alpha+\bar{\alpha})}+\beta\right]-6\alpha^2J_{351}+\frac{8\alpha(\bar{\alpha}^2-\alpha\beta)}{5}(J_{553}'-J_{551})\right\}\right),\quad\text{(A.20)}$$

$$G_{16}^{1}=-V_{LS}\left(\Gamma\left(\frac{3\pi^2}{2\alpha}\right)^{\frac{3}{2}}\left(\frac{1}{\sigma+18\lambda}\right)^{\frac{5}{2}}\left\{(15\alpha+9\bar{\alpha})J_{442}\left[\frac{\omega+\lambda(34\alpha+12\bar{\alpha})}{\sigma+18\lambda}+\beta,\right.\right.\right.$$
$$\left.\left.\left.-\frac{\xi+\lambda(8\alpha+24\bar{\alpha})}{\sigma+18\lambda},\frac{\omega+\lambda(10\alpha+12\bar{\alpha})}{\sigma+18\lambda}+\beta\right]+(3\alpha-9\bar{\alpha})J_{351}+\frac{12\alpha^2-4\alpha\bar{\alpha}+4\alpha\beta-12\bar{\alpha}\beta}{5}(J_{553}-J_{551})\right\}\right),\quad\text{(A.21)}$$

$$G_{26}^{1}=-V_{LS}\left(\Gamma\left(\frac{3\pi^2}{2}\right)^{\frac{3}{2}}\left[\frac{1}{\alpha\sigma+6\lambda(\alpha+\bar{\alpha})}\right]^{\frac{5}{2}}\left\{9\alpha(\alpha+\bar{\alpha})J_{442}\left[\frac{\alpha\omega+2\lambda(\alpha+\bar{\alpha})(6\alpha+\bar{\alpha})}{\alpha\sigma+6\lambda(\alpha+\bar{\alpha})}+\beta,-\frac{\alpha\xi-2\lambda(\alpha+\bar{\alpha})(6\alpha-2\bar{\alpha})}{\alpha\sigma+6\lambda(\alpha+\bar{\alpha})},\right.\right.\right.$$
$$\left.\left.\left.\frac{\alpha\omega+2\lambda(\alpha+\bar{\alpha})(6\alpha+\bar{\alpha})}{\alpha\sigma+6\lambda(\alpha+\bar{\alpha})}+\beta\right]+9\alpha(\alpha+\bar{\alpha})J_{351}+\frac{2\alpha[6\beta(\alpha+\bar{\alpha})-(2\alpha^2+6\alpha\bar{\alpha}+4\bar{\alpha}^2)]}{5}(J_{553}-J_{551})\right\}\right),\quad\text{(A.22)}$$

$$G_{15}^{2}=-V_{LS}\left(\Gamma\left[\frac{3\pi^2}{2(\alpha+\bar{\alpha})}\right]^{\frac{3}{2}}\left(\frac{1}{3\alpha+3\bar{\alpha}+6\lambda}\right)^{\frac{5}{2}}\left\{3(\alpha+\bar{\alpha})J_{442}\left[\frac{5\alpha(\alpha+\bar{\alpha})+2\lambda(6\alpha+\bar{\alpha})}{3\alpha+3\bar{\alpha}+6\lambda}+\beta,\right.\right.\right.$$
$$\left.\left.\left.\frac{8\alpha(\alpha+\bar{\alpha})+\lambda(12\alpha-4\bar{\alpha})}{3\alpha+3\bar{\alpha}+6\lambda},\frac{5\alpha(\alpha+\bar{\alpha})+2\lambda(6\alpha+\bar{\alpha})}{3\alpha+3\bar{\alpha}+6\lambda}+\beta\right]-3(\alpha+\bar{\alpha})J_{351}+\frac{4(\alpha-\beta)(\alpha+\bar{\alpha})}{5}(J_{553}-J_{551})\right\}\right),\quad\text{(A.23)}$$

where the superscripts 0, 1 and 2 refer to no-exchange, one-exchange and two-exchange, respectively. In Eqs. (A.18)–(A.23), we have omitted, for the sake of brevity, the arguments of some of the functions. In those cases, it is then understood that the arguments are identical with those expressed explicitly in the same equations.