Six-body hyperspherical solution to ^{6}Li bound states

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(Received 3 February 1978; revised manuscript received 10 May 1978)

We apply the hyperspherical method to the N-body Schrödinger equation and solve for the bound states of ^{6}Li with the center of mass motion correctly treated. It is shown how to construct antisymmetric hyperharmonic polynomials of definite J, J_z, T, and T_z from Slater determinants with shell model coordinates. A set of coupled one dimensional differential equations are obtained and solved in K_{min} approximation. A super-soft- core potential that provides a good fit to the two-nucleon scattering phase shifts is given a slight state dependence and is used for the two-nucleon potential. The proper handling of the potential energy matrix element with the center of mass motion excluded is detailed. A prescription for obtaining effective interactions for shell model calculations is presented. The difference in the potential energy matrix element of four $S_{1/2}$ nucleons in a ^{4}He nucleus or in a ^{6}Li nucleus is shown not to be zero. A J, $T = 1$, 1 state of ^{6}Li is calculated to have a binding energy of 15.245 MeV. This state may resemble a nuclear molecule of ^{3}H and ^{3}He.

[NUCLEAR STRUCTURE Many-body problem, hyperspherical method, ^{6}Li bound states.]

I. INTRODUCTION

We study bound state solutions of the N-body nucleus using the hypersphere[1] or K harmonic method. This method properly treats the nonrelativistic kinetic energy, and excludes the center of mass motion, which is important for small nuclei. The method has been applied[2,3] to the three-nucleon bound state problem using realistic two-nucleon potentials. The method has also been applied to $N=4$ problems,[4] the α particle, and the bound four neutron case, and the $J=0$ breathing mode of ^{16}O, but only in the approximation where K is restricted to K_{min}, its minimum value consistent with antisymmetrization requirements. The method has also[5,6] been applied to the ground state of ^{16}O. In the ^{3}He or ^{4}He bound state problems, the extension of the hypersphere method to more complex nuclei is not fully visible, as antisymmetric wave functions are obtainable from straight forward spin and isospin considerations. In spite of the problems encountered in explaining the states of these ^{3}He and ^{4}He isotopes, we characterize their spectra as simple, compared to the spectra of larger, more complex nuclei. For instance, the three-nucleon problem has only one bound state available for study. No evidence[7] for a bound excited state of ^{4}He exists. Excited states exist, with an excitation energy greater or equal to 20.1 MeV, but these states are unstable to proton emission. ^{6}He and ^{6}Li are the next simplest nuclei, as no stable $N=5$ nuclei exist.

^{6}Li has five excited states[8] with an excitation energy less than 6 MeV. The highest of these states undergoes decay into an α and a deuteron. The first four excited states have measurable electromagnetic decay widths.[8] The electromagnetic form factors for the ground and first excited state are also known.[9] Thus it is appropriate to treat these states as stable to nucleon decay, and to apply bound state boundary conditions in seeking their wave functions.

Thus ^{6}Li offers a complex spectra, characteristic of the rest of the (larger) nuclei. We view ^{6}Li as the simplest of the complex nuclei. Furthermore, spin and isospin considerations alone will not provide an antisymmetric wave function for this nucleus, as can be done for smaller nuclei. Antisymmetry of the wave function is guaranteed in ^{6}Li by use of a linear combination of Slater determinants as is done for larger nuclei. The similarities and differences of the Slater determinants used in the shell model and in the K harmonic method are spelled out in the next section.

The success of the shell model is principally for large nuclei and for states of low excitation. One possible reason for this limitation of the shell model is the introduction of spurious states by improper treatment of the center of mass motion. The convergence of the K harmonic method in K_{min} approximation can be correlated[10] to the existence of shell-like properties for larger nuclei. The rate of convergence of the method is unknown for ^{6}Li, but it may well be faster than in the three-nucleon problem.[2,3,5] Therefore, we report here on applying the K harmonic method to ^{6}Li as a six-body problem, using realistic two-nucleon potentials in the K_{min} approximation.

A three-body model where ^{6}Li is assumed to

consist of an α, a neutron, and a proton has been used previously to study the bound states by Wackman and Austern,[11] Barsella,[12] Shah and Mitra,[13] Rai *et al.*,[14] and by Fang and Tomusiak.[15] These calculations employed either a variational treatment or the Faddeev three-body formalism and have shown reasonable agreement with experimental binding energies. Other calculations by Dawson and Walecka,[16] Hauge and Maripuu,[17] and by Lodhi,[18] have employed the shell model to study ^{6}Li. These calculations have employed a system containing a doubly magic core plus two nucleons. A Bethe-Goldstone equation was solved[16] for the two external nucleons, and using the Brueckner-Gammel-Thaler potential, and binding energies and matrix elements were then found. Later work[17] used the effective Sussex interaction resulting in reasonable predictions of energy levels, or addressed[18] the question of the effect of two-nucleon correlations in the shell model wave function.

The shell model is the most microscopic of the nuclear models used to date for ^{6}Li. In this model the nucleus is considered as a system of nucleons moving in a common potential well arising from their mutual interactions.[19] We reject this independent particle shell model for ^{6}Li and instead use an opposite idea to describe the structure of the nucleus. We regard ^{6}Li as a strongly coupled nucleus in which the constituent motion of all the nucleons jointly plays an important part. Therefore, we will use the hyperspherical harmonics in a $K_{\min}$ expansion of the bound state wave function of ^{6}Li. Fang and Tomusiak[15] have previously used this expansion in a three-body model of ^{6}Li. The difference here is that we treat ^{6}Li as three protons and three neutrons not as an α, a neutron, and a proton. This work follows more along the lines of Simonov,[20] Baz and Zhukov,[21] Fabre de la Ripelle,[22] and Sadovoi.[10] We work directly with a two-nucleon potential and, therefore, cannot handle the infinities associated with hard core potentials. We will use and modify the *"dTS"* super-soft-core potentials of Cote, de Tourreil, Rouben, and Sprung[23] as they provide an excellent fit to the scattering phase shifts and have a short range core repulsion that is finite, not infinite.

The hyperspherical expansion reduces the Schrödinger equation to a set of possibly coupled differential equations to be solved for each set of quantum numbers: spin, isospin, and parity. We will work with jj coupled[24] states, as opposed to L, S coupled states. In $K_{\min}$, the possible configurations are

(a) $S_{1/2}{}^4P_{3/2}{}^2$

named 3, for $2j$ of each nucleon in the open shell,

(b) $S_{1/2}{}^4P_{3/2}P_{1/2}$

named 2, and

(c) $S_{1/2}{}^4P_{1/2}{}^2$

named 1.

The 1^+, $T=0$ ground state of ^{6}Li then requires the solution of a coupled set of equations involving all three configurations. The 3^+, $T=0$ first excited state of ^{6}Li, with excitation energy 2.185 MeV, involves solving an uncoupled equation using only the 3 configuration. The 0^+, $T=1$ second excited state involves solving a coupled set of equations using configurations 3 and 1 only. We consistently neglect the Coulomb potential throughout. Including the Coulomb potential would require four configurations to describe the 1^+ ground state wave function, rather than three, as a $P_{3/2}$ proton would be distinct from a $P_{3/2}$ neutron, and a $P_{1/2}$ proton would be distinct from a $P_{1/2}$ neutron. Then the 2 configuration would be replaced by two configurations, a $2pn$ and a $2np$ configuration.

The description of the hyperspherical or K harmonic approach to solving the six-body problem is arranged according to the following format. In Sec. II the method will be introduced, the geometry developed, and a way to construct the antisymmetric harmonic polynomials in $K_{\min}$ from combinations of Slater determinants will be given. This is followed by a detailed analysis of the $K_{\min}$ wave function for ^{6}Li. The details of evaluating the potential energy matrix element in the K harmonic expansion will then be presented. Numerical solution of the coupled differential equations one has to solve for the binding energy will be given in Sec. III. The required matrix elements of the two-nucleon potential used, and the solution to the differential equations obtained from a modified potential are described in Sec. IV. We conclude with a discussion of core polarization and of effective interactions in Sec. V, followed by a brief summary.

II. DETAILS OF THE K HARMONIC METHOD

A. Coordinates and geometric considerations

In the K harmonics method, one assumes the angular quantum numbers for the nucleons, just as in the shell model. However, one does not assume a radial wave function for each nucleon. Instead, one obtains a possibly coupled set of differential equations to be solved for the hyperradial part of the wave function and for the total binding energy of the nucleus. The intrinsic hyperspherical coordinates consist of a hyperradius and a set of $3N$-4 angular coordinates, where N is the number of nucleons. These angular coordinates, in addition to the spin and isospin coordinates, we denote by Ω. The hyper-radius is defined in terms of single particle coordinates

$\vec{r}_i$ by

$$\rho^2 = \sum_{i=1}^{N} (\vec{r}_i - \vec{R})^2 , \tag{1}$$

where $\vec{R}$ is the center of mass coordinate. We expand the many-body wave function ψ, in terms of harmonic polynomials Y_{ka} as

$$\psi = \frac{1}{\rho^{(3N-4)/2}} \sum_{ka} \chi_{ka} \, Y_{ka} . \tag{2}$$

Here a denotes the other quantum numbers needed to specify the state, for instance, the orbital quantum numbers. The Y_{ka} are orthonormalized and can be expressed in terms of a superposition of Slater determinants. The power of ρ in Eq. (2) is to simplify the coupled set of radial equations one must solve for the total energy E of the nucleus. The method is based on the nonrelativistic Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_{\vec{r}_i}^2 + \sum_{i<j}^{N} V_{ij} - E \right) \psi(1, 2, \ldots, N) = 0 , \tag{3}$$

where V_{ij} is the interaction between the ith and the jth nucleons. This interaction is assumed to be the same or nearly the same as that between two free nonrelativistic scattering nucleons. As written, Eq. (3) has the kinetic energy of the center of mass included. It is important to separate off the motion of the total center of mass at this point. To do this, we go over from the coordinates $\vec{r}_i$ to the Jacobi coordinates $\vec{\xi}_l$ and the coordinate of the center of mass $\vec{R}$,

$$\begin{aligned} &\vec{R} = \frac{1}{N} \sum_{i=1}^{N} \vec{r}_i , \\ &\vec{\xi}_l = \frac{1}{[l(l+1)]^{1/2}} \left(\sum_{j=1}^{l} \vec{r}_j - l\vec{r}_{l+1} \right) , \\ &\text{for } l = 1, 2 \ldots (N-1) . \end{aligned} \tag{4}$$

We note here the relation between the volume elements:

$$\begin{aligned} d\tau_{3N} &= \prod_{i=1}^{N} d\vec{r}_i \\ &= N^{3/2} d\vec{R} \prod_{j=1}^{N-1} d\vec{\xi}_j \\ &= N^{3/2} d\vec{R} \, d\vec{\tau}_{3(N-1)} . \end{aligned} \tag{5}$$

The set of $3(N-1)$ components of the vectors $\vec{\xi}_l$ can be regarded as components of a single vector in a $3(N-1)$ dimensional space spanned by the vectors $\hat{\xi}_l$. With the aid of Eq. (4), we obtain for the square of the hyper-radius, the relations

$$\begin{aligned} \rho^2 &= \sum_{i=1}^{N} (\vec{r}_i - \vec{R})^2 \\ &= \sum_{l=1}^{N-1} \xi_l^2 \\ &= \frac{1}{N} \sum_{i>j}^{N} (\vec{r}_i - \vec{r}_j)^2 \\ &= \sum_{i=1}^{N} r_i^2 - NR^2 . \end{aligned} \tag{6}$$

The volume element of this $3(N-1)$ dimensional space can be written as

$$d\vec{\tau}_{3(N-1)} = \prod_{l=1}^{N-1} d\vec{\xi}_l = \rho^{3N-4} d\rho d\Omega_\rho . \tag{7}$$

Here Ω_ρ denotes the set of $(3N-4)$ angles defining the direction of the vector $\vec{\rho}$ in the $(3N-3)$ dimensional space. Ω_ρ, plus the N spin and N isospin coordinates, we collectively denote by Ω. The purpose of these Jacobi coordinates is to separate out the center of mass motion. In these Jacobi coordinates, the Laplace operator separates as

$$\begin{aligned} \Delta_{3N} = \Delta_r &= \nabla_{r_1}^2 + \nabla_{r_2}^2 + \cdots + \nabla_{r_N}^2 \\ &= \Delta_\xi + \frac{1}{N} \nabla_R^2 , \end{aligned} \tag{8}$$

where

$$\Delta_\xi = \nabla_{\xi_1}^2 + \nabla_{\xi_2}^2 + \cdots + \nabla_{\xi_{N-1}}^2 . \tag{9}$$

Thus the use of Jacobi coordinates, Eq. (4), allows the kinetic energy associated with the center of mass motion to be separated out in the Hamiltonian. Using Eq. (8) in Eq. (3), and subtracting out the center of mass kinetic energy, results in the N-body Schrödinger equation with the center of mass motion removed

$$\left(-\frac{\hbar^2}{2m} \Delta_\xi + \sum_{i<j}^{N} V(\rho, \Omega) - E \right) \psi = 0 . \tag{10}$$

Here m is the average of the neutron and proton masses and not the reduced mass commonly encountered in two-body problems. E is the total energy of the nucleus in the center of mass frame. E is negative if the nucleus is bound. We have indicated the potential to be a function of space, spin, and isospin.

We now write Δ_ξ as

$$\Delta_\xi = \frac{d^2}{d\rho^2} + \frac{3N-4}{\rho} \frac{d}{d\rho} + \frac{L^2(\Omega\rho)}{\rho^2} , \tag{11}$$

separating the hyperspace Laplacian into its radial and angular parts. L^2, the angular part of the $3N-3$ dimensional space Laplacian will have eigenfunctions satisfying

$$L^2 Y_{ka} = -K(K+3N-5) Y_{ka} . \tag{12}$$

The wave function in Eq. (10) depends on the coordinates ρ, Ω, and we therefore expand the wave function as

$$\psi(\rho, \Omega) = \sum_{ka} R_{ka}(\rho) Y_{ka}(\Omega) . \tag{13}$$

The Y_{ka} will be orthonormalized functions. This separates the hyper-radial from the angular dependence in the wave functions and is analogous to the partial wave expansion in the two-body case. Substituting Eq. (13) and Eq. (11) into Eq. (10) results in equations describing the hyper-radial dependence of the wave function

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{d\rho^2}+\frac{3N-4}{\rho}\frac{d}{d\rho}-\frac{K(K+3N-5)}{\rho^2}\right)R_{ka}+(W^{ka}_{ka}-E)R_{ka}=-\sum_{k'a'\neq ka}^{\infty} W^{ka}_{k'a'}R_{k'a'}, \tag{14}$$

where

$$W^{ka}_{k'a'} = \int d\Omega\, Y^*_{k'a'} \sum_{i>j}^{N} V_{ij}(\rho, \Omega) Y_{ka} . \tag{15}$$

We have written the potential as a function of ρ, Ω as it is assumed to be spin and isospin dependent. The radial dependence can be expressed via Eq. (4) in the Jacobi coordinates.

The first derivative term in Eq. (14) can be eliminated by defining

$$R_{ka}(\rho) = \frac{\chi_{ka}(\rho)}{\rho^{(3N-4)/2}} . \tag{16}$$

Therefore, we expand the N-body wave function in the center of mass frame as

$$\psi(\rho, \Omega) = \frac{1}{\rho^{(3N-4)/2}} \sum_{ka}^{\infty} \chi_{ka}(\rho) Y_{ka}(\Omega) , \tag{2}$$

and obtain from Eqs. (14) and (16), the set of equations for $\chi_{ka}(\rho)$

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{d\rho^2}\chi_{ka}(\rho)-\frac{\mathfrak{L}(\mathfrak{L}+1)}{\rho^2}\chi_{ka}\right)+(W^{ka}_{ka}-E)\chi_{ka}(\rho)=-\sum_{k'a'\neq ka}^{\infty} W^{ka}_{k'a'}\chi_{k'a'}(\rho), \tag{17}$$

where

$$\mathfrak{L} = K + \tfrac{3}{2}(N-2) . \tag{18}$$

These equations are a set of coupled one dimensional equations that are to be solved for the unknown energy E and for the unknown hyper-radial functions $\chi_{ka}(\rho)$. K is related to the eigenvalue of the angular Laplace operator. For ground states or states of low excitation, hyper-radial functions with K equal to its minimum value are expected to be dominant. This is so because of the angular momentum barrier in Eq. (17) depends on K. This barrier pushes out hyper-radial functions with large K, away from the hyperorigin, so that they do not influence the shape of the minimum K hyperfunctions significantly. The sum of K in Eq. (17) is, therefore, truncated to its minimum value compatible with antisymmetry and angular momentum requirements. The boundary conditions are that all $\chi_{ka}(\rho)$ vanish as ρ approaches zero or infinity, for all ka. Thus each state is treated as a bound stable state that does not decay.

We now turn to the description of the $Y_{ka}(\Omega)$. The notation in the following is based on the earlier works of Siminov,[20] Baz and Zhukov,[21] and Fabre de la Ripelle.[22] Suppose we have a homogeneous polynomial P_{ka} of degree k, which satisfies

$$\Delta_\xi P_{ka} = 0 . \tag{19}$$

Then we can equate, subject to a future normalization, factor B,

$$P_{ka} = \frac{\rho^k Y_{ka}(\Omega)}{B} . \tag{20}$$

This is so because if P satisfies Eq. (19), then from Eqs. (11) and (20), we have

$$\left(\frac{d^2}{d\rho^2}+\frac{3N-4}{\rho}\frac{d}{d\rho}+\frac{L^2(\Omega\rho)}{\rho^2}\right)\rho^k Y_{ka}=0, \tag{21}$$

or

$$\frac{K(K-1)}{\rho^2}\rho^k Y_{ka}+\frac{(3N-4)K}{\rho^2}\rho^k Y_{ka} + \frac{L^2(\Omega\rho)}{\rho^2}\rho^k Y_{ka}=0 . \tag{22}$$

From this we see that Y_{ka} then must satisfy

$$L^2(\Omega\rho) Y_{ka} = -K(K+3N-5) Y_{ka} . \tag{23}$$

So if we can satisfy Eq. (19), using Eq. (20), Eq.

(23) will be satisfied. Thus a polynomial of degree k which satisfies Eq. (19), when divided by ρ^k, is an eigenfunction of Eq. (23). Now $\chi_{ka}(\rho)$ is a completely symmetric function upon exchange of nucleon coordinates, as ρ is a completely symmetric function [see Eq. (6)]. Thus, we must demand that Y_{ka} and P_{ka} be completely antisymmetric functions, upon the exchange of any pair of nucleon coordinates. Coordinates here must include spin and isospin, as well as space coordinates. The shell model (SM) satisfies this antisymmetry requirement by using a Slater determinant of basis functions ϕ. These basis functions can be chosen as eigenfunctions of an appropriate one-body Hamiltonian. We write the shell model solution as

$$\psi_{\rm SM}(1,2,\ldots,N)=\frac{1}{\sqrt{N!}}\det\begin{vmatrix}\phi_1(\vec{r}_1) & \phi_1(\vec{r}_2) & \cdots & \phi_1(\vec{r}_N)\\ \phi_2(\vec{r}_1) & \phi_2(\vec{r}_2) & \cdots & \phi_2(\vec{r}_N)\\ \vdots & \vdots & & \vdots\\ \phi_2(\vec{r}_1) & \phi_N(\vec{r}_2) & \cdots & \phi_N(\vec{r}_N)\end{vmatrix}. \tag{24}$$

The normalization and volume of integration are indicated by

$$\int \psi^*_{\rm SM}\,\psi_{\rm SM}\,d\tau_{3N}=1. \tag{25}$$

Here the integration over spin and isospin coordinates is understood. Note all N coordinates $\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N$ are treated as independent variables in the shell model.

In the K harmonics method, we wish to construct a completely antisymmetric eigenfunction (polynomial) using the $3N-3$ ρ, Ω_ρ coordinates, plus the $2N$ spin-isospin coordinates. The K harmonics solution to the N-body problem has three major parts. The first is the construction of the K harmonic wave function of proper antisymmetry, the Y_{ka} needed in Eq. (13). The second problem is the evaluation of the potential energy matrix elements indicated in Eq. (15) which are needed to solve for the unknown hyper-radial functions. The third part is the numerical solution of the truncated coupled set of equations for the hyper-radial dependence, Eq. (14). We now undertake the resolution of these problems.

We want to construct an antisymmetric polynomial upon exchange of any pair of nucleons coordinates. The Jacobi coordinates are inconvenient for this task because of their complicated transformation laws under permutations. We, therefore, tentatively use the coordinates of the nucleons reckoned from their common center of mass

$$\vec{\rho}_i=\vec{r}_i-\vec{R},\quad i=1,\ 2,\ldots,N, \tag{26}$$

where $\vec{\rho}_i$ are the center of mass nucleon coordinates commonly used in the shell model. They are not independent, because they satisfy the relation

$$\sum_{i=1}^{N}\vec{\rho}_i=0. \tag{27}$$

The result of permutations on these coordinates is obvious, but we note the Laplacian does not separate in these coordinates. We wish to find an antisymmetric polynomial which satisfies the equation

$$\Delta_\xi P(\vec{\rho}_i)=0. \tag{28}$$

Analogous to the shell model, we construct the one-body basis function of one variable $\vec{\rho}_i$

$$\Phi_{\omega_p}(i)\equiv C_{n_p l_p}(\rho_i)^{2n_p+l_p}Y_{l_p m_p}(\hat{\rho}_i)\,\alpha_{\mu_p\tau_p}(i), \tag{29}$$

where

$$C_{nl}=(-1)^n\sqrt{2}\,[\Gamma(n+1)\Gamma(n+l+\tfrac{3}{2})]^{-1/2}. \tag{30}$$

Here $Y_{lm}(\hat{\rho})$ is the usual spherical harmonic, $\alpha_{\mu\tau}$ is the spin-isospin wave function for the ith nucleon with spin and isospin projections μ and τ. The exponent n can take on nonnegative interger values. We will use the lower index ω_p of Φ_{ω_p} to denote the set of all five quantum numbers $\{n,l,m,\mu,\tau\}$. In the following we shall label the state of a nucleon by these numbers. We now form an N by N Slater determinant of the basis functions Φ_{ω_i}

$$P(\vec{\rho}_1,\vec{\rho}_2,\ldots,\vec{\rho}_N)=\det\begin{vmatrix}\Phi_{\omega_1}(1) & \Phi_{\omega_1}(2) & \cdots & \Phi_{\omega_1}(N)\\ \Phi_{\omega_2}(1) & \Phi_{\omega_2}(2) & \cdots & \Phi_{\omega_2}(N)\\ \cdot & \cdot & & \cdot\\ \cdot & \cdot & & \cdot\\ \cdot & \cdot & & \cdot\\ \Phi_{\omega_n}(1) & \Phi_{\omega_n}(2) & & \Phi_{\omega_n}(N)\end{vmatrix}. \tag{31}$$

This corresponds to the m scheme shell model wave function. The degree of the basis function is equal to $2n+l$. Then the degree of the polynomial formed from the determinant is

$$K=\sum_{p=1}^{N}(2n_p+l_p). \tag{32}$$

We adopt a prescription for selecting the values of n and l when choosing the basis functions to form the determinant that agrees exactly with the prescription for the lowest configuration of the shell model. Namely, the lowest value of $(2n+l)$ is used successively until m, μ, and τ have exhausted all their possible sets of values, then $(2n+l)$ is increased, etc. The value of K determined from Eq. (32), when the determinant is formed following this prescription we call $K_{\min}$. The Slater determinant P formed in this manner is a homogeneous antisymmetric polynomial of minimal degree $K_{\min}$. If the degree K of the polynomial were any smaller, then two of the basis functions in the Slater determinant would be identical, and the Slater determinant would vanish. Therefore, the $K_{\min}$ degree polynomial formed must necessarily be harmonic; that is, it must obey Eq. (19) which we write as

$$\Delta_\xi P_{k_{\min}}(\vec{\rho}_i)=0. \tag{33}$$

To prove[20] Eq. (33), we note that $P_{k_{\min}}$ depends on the $\vec{\rho}_i$ which can be expressed through the Jacobi variables via Eq. (4) and (26); and, therefore, the action of the Laplacian Δ_ξ leads to a lowering of the degree K of the polynomial by two, that is

$$\Delta_\xi P_{k_{\min}}=P_{k_{\min}-2}. \tag{34}$$

On the other hand, the operator Δ_ξ is completely symmetric and, therefore, $\Delta_\xi P_{k_{\min}}$ is again an antisymmetric polynomial. Since there is no nonvanishing antisymmetric polynomial of degree $K_{\min}-2$, Eq. (33) must be true.

The polynomials $P_{K_{\min}}$ depend on the coordinates $\vec{\rho}_i$; and, therefore, the motion of the center of mass is excluded from them. This means we must remember to take into account in Eq. (31) that

$$\sum_{i=1}^{N}\vec{\rho}_i=0. \tag{27}$$

However, it is easy to prove[20] for the polynomials $P_{k_{\min}}$, that

$$P_{k_{\min}}(\vec{\rho}_i)=P_{k_{\min}}(\vec{\rho}_i+R)=P_{k\min}(\vec{r}_i). \tag{35}$$

If one expands $P_{k_{\min}}(\vec{\rho}_i+\vec{R})$ in a sum of polynomials of $\vec{\rho}_i$ with coefficients depending on powers of $\vec{R}$, the polynomials of $\vec{\rho}_i$ will be antisymmetric because of the symmetry of $\vec{R}$, see Eq. (4), and they will have a degree lower than $K_{\min}$, and all will vanish, therefore, except the coefficient of R to the zero power. Hence $P_{k_{\min}}(\vec{\rho}_i)=P_{k_{\min}}(\vec{\rho}_i+\vec{R})$ is indeed independent of $\vec{R}$. This means we can use, at least in a $K_{\min}$ calculation, Slater determinants where the basis functions are expressed as functions of $\vec{r}_i$, as in the shell model, or as functions of $\vec{\rho}_i$, whichever is more convenient for calculations. Equation (35) shows that either form satisfies Eq. (19), and so is a harmonic polynomial. We note that Eq. (15) requires an integral $d\Omega_\rho$ over $3N-4$ space angles to evaluate the potential energy matrix elements, rather than an integration over $d\tau_{3N}$ as in the shell model. The differences in these volumes of integration are seen by comparing Eq. (5) and (7). How to perform the integration for Eq. (15) will be shown later in this section.

B. Wave functions for ^{6}Li

We have indicated in Sec. II A how to construct polynomials in the m scheme that are harmonic and antisymmetric. We now wish to convert to the j, jz coupling scheme[24-26]. To do this, instead of using basis functions indicated in Eq. (29), we use linear combinations of them coupled to a definite j, jz,

$$\Phi_{(n_p j_p l_p j_{zp}\tau_p)}(i)=\sum_{m_p\mu_p}\Phi_{(n_p l_p m_p \mu_p \tau_p)}\langle l_p m_p \tfrac{1}{2}\mu_p | j_p j_{\xi p}\rangle. \tag{36}$$

We now denote the state of a nucleon by the set of quantum numbers

$$\omega_p=\{n_p, j_p, l_p, j_{zp}, \tau_{zp}\}, \tag{37}$$

rather than using the m scheme. We consider the states of ^{6}Li to have a definite total spin J, and a definite total isospin, T. We can form a K harmonic wave function with these definite total J, T values, by constructing linear combinations of the m scheme determinants. We denote such a harmonic as $Y_{k\alpha}^{JT}$, where α is the set of all remaining quantum numbers characterizing the nuclear state. Using a j, j_z coupled set of basis functions, in $K_{\min}$ approximation, there are three configurations or three sets of quantum numbers "α." For $K_{\min}$ calculations, all the n values describing each nucleon are zero. Hence, the n values are omitted in what follows, as they never change from zero. The $K_{\min}$ configurations for ^{6}Li are

A $(S_{1/2})^4(P_{3/2})^2$ named 3,
B $(S_{1/2})^4(P_{3/2}P_{1/2})$ named 2,
C $(S_{1/2})^4(P_{1/2})^2$ named 1.

This labeling of the configurations indicates the usual shell model n, l, j quantum numbers assigned to each of the six nucleons in ^{6}Li. The j_z, t_z values

have not been indicated here. Let us label the associated Slater determinants constructed using the basis functions, Eq. (36), indicating the j_z, t_z values for the unfilled shell nucleons, by the following:

$P_{33}^{m_5 m_6 t_5 t_6}$ when using the basis functions of set A,

$P_{31}^{m_5 m_6 t_5 t_6}$ when using the basis functions of set B, and

$P_{11}^{m_5 m_6 t_5 t_6}$ when using the basis function of set C.

Here we have explicitly indicated the dependence of the Slater determinants on the j_z and t_z values of the nonclosed-shell nucleons. We are now dealing with basis functions that have a definite j, j_z, but the determinant itself does not have a definite total J, J_z, T, or T_z. This is accomplished by taking linear combinations of these Slater determinants, with coefficients that are Clebsch-Gordan coefficients, coupling to definite total J, J_z, T, and T_z. The ground state of ^{6}Li has J equal to one, and isospin T equal to zero. Therefore, in $K_{\min}$ approximation we take the ground state wave function to be

$$\psi^{JMT,O} = \frac{B\sum}{\rho^{k+(3N-4)/2}} \begin{aligned} &\chi_{33}(\rho)\langle \tfrac{3}{2} m_5 \tfrac{3}{2} m_6 | JM\rangle \langle \tfrac{1}{2} t_5 \tfrac{1}{2} t_6 | TO\rangle P_{33}^{m_5 m_6 t_5 t_6} \\ &+\chi_{31}(\rho)\langle \tfrac{1}{2} m_6 \tfrac{3}{2} m_6 | JM\rangle \langle \tfrac{1}{2} t_5 \tfrac{3}{2} t_6 | TO\rangle P_{31}^{m_5 m_6 t_5 t_6} \\ &+\chi_{11}(\rho)\langle \tfrac{1}{2} t_5 \tfrac{1}{2} t_6 | JM\rangle \langle \tfrac{1}{2} t_5 \tfrac{1}{2} t_6 | TO\rangle P_{11}^{m_5 m_6 t_5 t_6} . \end{aligned} \tag{38}$$

The summation is over m_5, m_6, t_5, and t_6. We have used Eq. (20) with Eq. (2) and have constructed a state of definite J, M, T, and $T_z = 0$ from the three possible sets of Slater determinants. The $K_{\min}$ approximation neglects all determinants with higher values of K than $K_{\min}$, which is two for ^{6}Li. B is a normalization constant that will be determined later, see Eq. (56).

In general not every one of the three sets of Slater determinants will contribute to a state of given J, T, depending on the particular value of J and T. Table I indicates the allowed states for ^{6}Li in a $K_{\min}$ calculation. A check there indicates a particular configuration is a nonvanishing part of the nuclear wave function. For future convenience, we define, from Eq. (38),

$$Y_{ka}^{JT} = \sum_{\substack{m_5 m_6 \\ t_5 t_6}} \langle \tfrac{3}{2} m_5 \tfrac{3}{2} m_6 | JM\rangle \langle \tfrac{1}{2} t_5 \tfrac{1}{2} t_6 | TO\rangle \frac{B P_{33}^{m_5 m_6 t_5 t_6}}{\rho^k} \quad \text{for } a = 33 \tag{39}$$

for each of the three values of a. We then have from Eq. (18),

$$\frac{-\hbar^2}{2m}\left(\frac{d^2}{d\rho^2}\chi_{ka}(\rho) - \frac{\mathcal{L}(\mathcal{L}+1)}{\rho^2}\chi_{ka}\right) + (W_{aa}^{JT} - E)\chi_{ka} = -\sum_{a' \neq a} W_{aa'}^{JT}\chi_{ka'}, \tag{40}$$

where

$$W_{aa'}^{JT} \equiv \int d\Omega\, Y_{ka'}^{*JT} \sum_{i<j}^{N} V_{ij}(\rho, \Omega) Y_{ka}^{JT} . \tag{41}$$

Thus we must evaluate the potential energy matrix elements for states with a definite J, M, T, and T_z, but the other quantum numbers are not necessarily diagonal. The potential energy matrix element is independent of M and T_z, as we neglect the Coulomb potential.

C. Evaluation of the potential energy matrix element

The evaluation of the potential energy matrix element parallels the shell model evaluation but is different in some details. We can analytically perform all but one of the integrals indicated in Eq. (41) for W_{aa}^{JT}, for a local potential that is every where finite. If the potential has a simple analytical form, such as a Yukawa or exponential dependence, then all the integrals can be done analytically. That is the type of potential we will utilize. Let us consider the integral first evaluated by Zurkov, according to Baz and Zhukov[21]:

TABLE I. Configurations contributing to possible ^{6}Li states.

J	T	$P_{3/2}^2$	$P_{3/2}P_{1/2}$	$P_{1/2}^2$
1	0	x	x	x
3	0	x		
0	1	x		x
2	0		x	
2	1	x	x	
1	1		x	

$$J \equiv \int G(\xi)d\Omega = \frac{1}{\pi i \rho^{3N-5}} \int_c ds \left(\frac{S}{\pi}\right)^{3/2} \exp\left[S\left(\rho^2 - \sum_{i=1}^{N} r_i^2\right)\right] G(\xi) d\tau_{3N}, \tag{42}$$

where $G(\xi)$ is translationally invariant, that is, it does not depend on the position R of the center of mass of the system. The contour integral ds is up the imaginary s axis from minus to plus infinity. $d\Omega$ includes a summation (understood) over the spin and isospin coordinates, which are assumed to be also included in $d\tau_{3N}$. We note two identities,

$$d\Omega = \delta\left(\rho^2 - \sum_{p=1}^{N-1} \xi_p^2\right) d\rho^2 d\Omega = \frac{2}{\rho^{3N-5}} \delta\left(\rho^2 - \sum_{p=1}^{N-1} \xi_p^2\right) d\tau_{3(N-1)}, \tag{43}$$

and

$$\left(\frac{u}{\pi}\right)^{3/2} \int e^{-uR^2} d\vec{R} = 1, \quad \text{for real } u > 0. \tag{44}$$

Combining these identities and using Eq. (43), J can be rewritten as

$$J = \frac{2}{\rho^{3N-5}} \int G(\xi) \left(\frac{u}{\pi}\right)^{3/2} e^{-uR^2} \delta\left(\rho^2 - \sum_{p=1}^{N-1} \xi_p^2\right) d\vec{R} d\tau_{3(N-1)}, \tag{45}$$

$$= \frac{2}{\rho^{3N-5}} \int G(\xi) \left(\frac{u}{N\pi}\right)^{3/2} e^{-uR^2} \delta\left(\rho^2 - \sum_{p=1}^{N-1} \xi_p^2\right) d\tau_{3N}. \tag{46}$$

We now use the integral representation[1] of the δ function,

$$\left(\frac{u}{N\pi}\right)^{3/2} e^{-uR^2} \delta\left(\rho^2 - \sum_{p=1}^{N-1} \xi_p^2\right) = \frac{1}{2\pi i} \int_c ds \left(\frac{u}{N\pi}\right)^{3/2} \exp\left[-uR^2 + S\left(\rho^2 - \sum_{p=1}^{N-1} \xi_p^2\right)\right]. \tag{47}$$

Since the parameter u in Eq. (44) is arbitrary, as long as real u is greater than zero, one can set $u = Ns$ into Eq. (47), which combines with Eq. (6) to prove Eq. (42). We now take G in Eq. (42) to be an arbitrary translational invariant operator Q, sandwiched between two $K = K_{\min}$, K harmonic wave functions. We then have

$$Q_{aa'}^{JT} = \int Y_{ka'}^{*JT}(\Omega) Q(\rho, \Omega) Y_{ka}^{JT}(\Omega) d\Omega$$

$$= \frac{1}{\pi i \rho^{3N-5}} \int_c ds \left(\frac{S}{\pi}\right)^{3/2} \exp\left[S\left(\rho^2 - \sum_{i=1}^{N} r_i^2\right)\right] \times Y_{ka'}^{*JT} Q Y_{ka}^{JT} d\tau_{3N}. \tag{48}$$

We transform the integrand in Eq. (48) using the following steps:

$$\exp\left(-\frac{S}{2}\sum_{i=1}^{N} r_i^2\right) Y_{ka}^{JT} = \frac{BS_4}{\rho^k \sqrt{N!}} \left[\sum_{i=1}^{N} \exp\left(-\frac{S}{2} r_i^2\right)\right] \times P_a^{m_5 m_6 t_5 t_6}$$

$$= \frac{BS_4}{\rho^k \sqrt{N!}} S^{-1/2k - 3N/4} \times \det|\tilde{\Phi}_{\omega_p}(j)|, \tag{49}$$

where

$$S_4 \equiv \sum_{m_5, m_6, \tau_5, \tau_6} \langle j_5 m_5 j_6 m_6 | JM \rangle \langle \tau_5 \tau z_6 \tau_6 \tau z_5 | T T_z \rangle \tag{50}$$

The sums, in Eq. (50), of products of Clebsch-Gordan coefficients are the same sums that appear in Eq. (39), where nuclear states of total J, M, T, and T_z are formed. S_4, refers to the same sums as in Eq. (50) except with all dummy indices replaced by their primed (′) values. In Eq. (49) we have also defined,

$$\tilde{\Phi}_\omega(j) = \sum_{m, \mu} R_{nl}^b(r_j) Y_{lm}(\hat{r}_j) \alpha_{\mu\tau}(j) \langle l\, m\, \tfrac{1}{2}\, \mu | J m_j \rangle, \tag{51}$$

where

$$R_{nl}^b(r) = b^{-3/2} [2\Gamma(n+1)\Gamma(n+l+3/2)]^{1/2} e^{-r^2/2b^2} \left(\frac{r}{b}\right)^{2n+l} \sum_{m=0}^{n} (-1)^m \frac{(r/b)^{2m-2n}}{\Gamma(m+1)\Gamma(n-m+1)\Gamma(m+l+3/2)}. \tag{52}$$

In these expressions, $b = S^{-1/2}$, and $R_n(x)$ is a harmonic oscillator wave function of order n and argument x. As a result of the transformation Eq. (49), we have obtained a Slater determinant constructed from basis functions $\tilde{\Phi}_\omega$, which are orthogonal in all five quantum numbers

$$\omega \equiv \{n, l, j, m, \tau\}. \tag{53}$$

The basis functions are also harmonic oscillator eigenfunctions with a complex (imaginary) argument. This property will be useful in the final reduction of the matrix element of the potential energy.

If the operator Q in Eq. (48) is set to unity, we obtain for the scalar product of two K harmonics

$$\begin{aligned}\int Y^{*JT}_{ka'} Y^{JT}_{da}\, d\Omega &= S_4 S_{4'} \int_c ds\, D(S,\rho^2) \\ &\quad \times \prod_{p=1}^{N} \left(\int d\vec{r}_j \tilde{\Phi}_{\omega_p}(j) \tilde{\Phi}_{\omega'_p}(j) \right) \\ &= \int ds\, D(S,\rho^2) \delta_{aa'} \\ &= \delta_{aa'} B^2 / [\pi^{3/2} \Gamma(K + 3(N-1)/2)], \end{aligned} \tag{54}$$

where

$$D(S,\rho^2) \equiv \frac{B^2 S^{-K-3N/2}}{\pi i \rho^{2K+3N-5}} \left(\frac{S}{\pi} \right)^{3/2} e^{S\rho^2}. \tag{55}$$

The symbol $\delta_{aa'}$ in this formula is equal to zero when $a = \{\{\omega_1, \omega_2, \ldots, \omega_N\}, J, M, T, T_z\}$ and a' differ in at least one value. If the sets a and a' coincide except for an ω permutation, then $\delta_{aa'} = \pm 1$, depending on the parity of the permutation. If J, M, T, or T_z were not identical in S_4 and $S_{4'}$, then the summations over the products of the Clebsch-Gordan coefficients will vanish. It follows that the normalization constant B in Eq. (39) for the K harmonic is equal to

$$B^2 = \pi^{3/2} \Gamma(K + 3(N-1)/2). \tag{56}$$

We now take the operator Q in Eq. (48) to be the potential energy. Then we have

$$\begin{aligned} W^{JT}_{aa'} &= \int Y^{*JT}_{ka'} \left(\sum_{i<j}^{N} V_{ij}(\rho, \Omega) \right) Y^{JT}_{ka} \\ &= \tfrac{1}{2} S_4 S_{4'} \int_c ds\, D(S,\rho^2) \{\det |\tilde{\Phi}_{\omega_p}(j)|\} \\ &\quad \times \sum_{i,j}^{N} V_{ij}(\rho, \Omega) \{\det |\tilde{\Phi}_{\omega'_p}(j)|\} \prod_{p=1}^{N} d\vec{r}_p. \end{aligned} \tag{57}$$

This expression is easily simplified using shell model techniques.[25,26] It is important to realize the harmonic oscillator basis functions now appear in the last of the above equations. They result from the transformations brought about by Eqs. (49)–(52). Standard techniques allow Eq. (57) to be reduced to two-body integrals in the shell model. Here we have in addition, the contour integral ds to be performed. However, the presence of harmonic oscillator basis functions allows one to use the Moshinsky bracket transform[27] to go from $\vec{r}_i, \vec{r}_j$ coordinates into relative and two-body center of mass coordinates $\vec{r}$ and $\vec{R}_{ij}$. The factor $\frac{1}{2}$ comes from removing the restriction $i<j$ in the summations. We evaluate the case when J, M, T, and T_z are identical in both S_4 and $S_{4'}$. Then when $a = a' = 3$, we obtain

$$\begin{aligned} W^{JT}_{aa} = \int ds\, D(S,\rho^2) \Bigg(&\sum_{i<j}^{c} \langle \tilde{\Phi}_{\omega_i} \tilde{\Phi}_{\omega_j} | V_{12} | \tilde{\Phi}_{\omega_i} \tilde{\Phi}_{\omega_j} - \tilde{\Phi}_{\omega_j} \tilde{\Phi}_{\omega_i} \rangle \\ &+ 2 \sum_{j}^{c} \langle \tilde{\Phi}_{\omega_6} \tilde{\Phi}_{\omega_j} | V_{12} | \tilde{\Phi}_{\omega_6} \tilde{\Phi}_{\omega_j} - \tilde{\Phi}_{\omega_j} \tilde{\Phi}_{\omega_6} \rangle \\ &+ S_4 S_{4'} \langle \Phi_{\omega_5} \Phi_{\omega_6} | V_{12} | \tilde{\Phi}_{\omega'_5} \tilde{\Phi}_{\omega'_6} - \tilde{\Phi}_{\omega'_6} \tilde{\Phi}_{\omega'_5} \rangle \Bigg). \end{aligned} \tag{58}$$

If a differs from a' by one single nucleon state, for example, $a = 3$, $a' = 2$, or if a differs from a' by two single nucleon states, for example, if $a = 3$, and $a' = 1$, then we obtain

$$\begin{aligned} W^{JT}_{aa'} \equiv &\int ds\, D(S,\rho^2) S_4 S_{4'} \\ &\times \langle \tilde{\Phi}_{\omega_5} \tilde{\Phi}_{\omega_6} | V_{12} | \tilde{\Phi}_{\omega'_5} \tilde{\Phi}_{\omega'_6} - \tilde{\Phi}_{\omega'_6} \tilde{\Phi}_{\omega'_5} \rangle. \end{aligned} \tag{59}$$

In the above expression, c the upper limit of the summation means to sum over the nucleons in the closed shells. Normally, the expressions obtained,[25] when one or two nucleon states differ, are not the same. However, for ^{6}Li, in $K_{\min}$, the difference vanishes for these two cases. The two nucleon matrix elements depend on the complex parameter s through the definition of the basis functions $\tilde{\Phi}_\omega$. Therefore, the two nucleon matrix elements cannot be taken outside the contour integral ds in Eqs. (58), (59). The sums implicit in $S_4, S_{4'}$ can be done analytically. The final results appear below in Eqs. (77)–(82) for ^{6}Li. As an approximation, we could perform the contour integration over ds by the method of steepest descent. Then we would obtain potential energy matrix elements identical in form to those found in the harmonic oscillator shell model, with an oscillator radius b given by

$$b = \rho [K + 3(N-1)/2]^{-1/2}, \tag{60}$$

and an oscillator frequency ν given by

$$\nu = (\hbar / m\rho^2)[K + 3(N-1)/2]. \tag{61}$$

We do not do the contour integral by the steepest descent method, see Eq. (74) below. In general, what is needed to evaluate Eq. (58) and (59) is

$$A \equiv \langle ijJT|V|klJT\rangle = \int ds\, D(S,\rho^2) \sum_{\substack{m_i m_j m_k m_l \\ \tau_i \tau_j \tau_k \tau_L}} \langle j_i m_i j_j m_j | JM\rangle \langle j_k m_k j_l m_l | JM\rangle \langle \tfrac{1}{2}\tau_i \tfrac{1}{2}\tau_j | TT_z\rangle \langle \tfrac{1}{2}\tau_k \tfrac{1}{2}\tau_l | TT_z\rangle$$

$$\times \langle \Phi_{\omega_i}\Phi_{\omega_j}|V_{12}|\Phi_{\omega_k}\Phi_{\omega_l}\rangle$$

minus the $k \leftrightarrow l$ term times $(-1)^{1+T+j_k+j_l+J}$. (62)

In Eq. (62) we are going over to an antisymmetrized isospin formalism where we assume the matrix element of the two nucleon interaction is independent of M and T_z. It does, however, depend on J, T, and the single nucleon quantum numbers (nlj) for nucleons i, j, k, and l, as indicated on the left-hand side of Eq. (62).

To proceed with the evaluation of A, one decouples the orbital angular momentum l, from the intrinsic spin, also called s, from j, the angular momentum for each nucleon wave function. As the radial part of the wave function matches that of a harmonic oscillator, one can immediately use the Moshinsky bracket transformation[27] into relative and two-body center of mass coordinates, from $\vec{r}_i$ and $\vec{r}_j$:

$$|r_i n_i l_i m l_i\rangle\, |r_j n_j l_j m l_j\rangle = \sum_{\substack{\lambda\lambda_z N L n l, \\ m M_L}} \langle l_i m l_i l_j m l_j | \lambda\lambda_z\rangle\, C^{nlNL}_{mosh} \times \langle lmLM_L|\lambda\lambda_z\rangle\, |rnlm\rangle\, |RNLM_L\rangle\,. \quad (63)$$

One can now do the integral dR_{12} obtaining dirac δ functions for the center of mass harmonic oscillator wave function quantum numbers N, L, and M_L. One still has the relative coordinate radial integral to do. This, when combined with the contour integral ds, we write as

$$B_r = \int_c \int_0^{\rho} H_{nl}(r) H_{n'l'}(r)\, V_{12}^{JTll'} \times (r_1 - r_2) r^2 dr\, D(S,\rho^2) ds\,. \quad (64)$$

The finite upper limit on dr comes from Eq. (47) where the δ function representation was introduced, requiring the coefficient of s in the exponential to be positive. The radial factors H are given by Eq. (52) in terms of b. Here we express them in terms of s, in a form convenient for the final integral evaluation. We have

$$H_{nl}(r) = S^{3/4} g_n e^{-Sr^2/2} (S^{1/2} r)^{2n+l} \sum_{m=0}^{n} h_{mn} (Sr^2)^{m-n}, \quad (65)$$

where

$$g_n = [2\Gamma(n+1)\Gamma(n+l+3/2)]^{1/2}, \quad (66)$$

and where we define

$$h_{mn} = (-1)^m / [\Gamma(m+1)\Gamma(n-m+1)\Gamma(m+l+\tfrac{3}{2})]. \quad (67)$$

We change variables from r to z, where $r^2 = z\rho^2$, so that z is dimensionless and ranges from zero to one. Using Eq. (55) for D, we obtain

$$B_r = \sum_{mm'}^{nn'} g_n g_{n'} h_{mn} h_{m'n'} \times \int_0^1 \frac{\rho^3 z^{1/2} dz\, V_{12}(\sqrt{2z}\,\rho) B^2 (z\rho^2)^x}{2\rho^{2k+3N-5}\pi^{3/2}\pi i} \times \int_c \frac{ds S^{3+x}}{S^{k+3N/2}} e^{S\rho^2(1-z)}, \quad (68)$$

where we define

$$x = m + m' + \tfrac{1}{2}(l + l'). \quad (69)$$

Now the contour integral can be done[1,22] as

$$\frac{1}{\pi i}\int_c \frac{ds\, e^{SY^2}}{S^{K-x-3+3N/2}} = \frac{Y^{2K+3N-8-2x}}{\Gamma(K - x + 3(n-2)/2)}. \quad (70)$$

Therefore the final integral we obtain is of the form

$$B_r = \sum_{mm'}^{nn'} \frac{g_n g_{n'} h_{mn} h_{m'n'} B^2}{2\pi^{3/2}\Gamma(q)} \times \int_0^1 z^{x+1/2}(1-z)^{q-1} V(2^{1/2}\rho z^{1/2}) dz, \quad (71)$$

where

$$q = k - x + 3(N-2)/2\,.$$

For the Sprung[23] super-soft-core potential we use, the potential is a sum of Yukawa-type terms, the coefficients depending on J, T, l, and l'. The potential is smoothed to a constant value below a given cutoff radius r_c. For this potential the integral dz can be done analytically, yielding E_n functions[28] or a sum of incomplete γ functions. The finite upper limit to the above integral is one of the major differences between the K harmonic and the shell model evaluation of the potential energy. For small ρ, the asymptotic tail of the potential has no bearing on the value of B_r. Only the potential from r = zero to $r = 2^{1/2}\rho$ contributes to the potential energy matrix element $W(\rho)$. Of course, as ρ approaches infinity, all regions of the two nucleon potential are included in B_r.

The decoupling of intrinsic spin and orbital angular momentum was necessary to get from Eq. (62) to (64). One can do a complete reduction of the resulting sums of Clebsch-Gordan coefficients into sums of $6j$ and $9j$ symbols. We obtain for Eq. (62)

$$A=\sum(-1)^{\lambda+\lambda'}C^{nlNL}_{mosh}C^{n'l'NL}_{mosh}B_r(\hat{j}_i\hat{j}_j\hat{j}_k\hat{j}_l\hat{S}\hat{S}')^{1/2}(\hat{\lambda}\hat{\lambda}'\hat{J}_{12})$$
$$\times\begin{bmatrix} j_i & j_l & J \\ \frac{1}{2} & \frac{1}{2} & S \\ l_i & l_j & \lambda \end{bmatrix}\begin{bmatrix} j_k & j_l & J \\ \frac{1}{2} & \frac{1}{2} & S' \\ l_k & l_l & \lambda' \end{bmatrix}\begin{Bmatrix} L & l & \lambda \\ S & J & J_{12} \end{Bmatrix}\begin{Bmatrix} L & l' & \lambda' \\ S' & J & J_{12} \end{Bmatrix}$$
$$\times[1-(-1)^P]. \tag{72}$$

Here we define

$$P=T+S+l_k+l_l+\lambda'. \tag{73}$$

The sum in Eq. (72) is over λ, λ', S, S', J_{12}, n, l, N, L, n', and l'. We also define $\hat{j}=2j+1$. The square brackets denote $9j$ symbols, and the curly brackets denote $6j$ symbols, and B_r is the radial part of the matrix element, given by Eqs. (66)–(71). The potential is diagonal in spin, so the sum over S' is redundant, as S' always equals S for the nonvanishing part of the potential.

We now do the sums implicit in S_4, S_4' appearing in Eqs. (58) and (59) and express the results in terms of

$$A=\langle ijJT|V|klJT\rangle, \tag{74}$$

given by Eq. (62). Here i, j, k, and l refer to only the n_il_i and j_i quantum numbers for the nucleon i, etc. The mutual interaction of a group of nucleons, all in closed shells, can then be written

$$A_{CC}=\tfrac{1}{2}\sum_{i,j}^{\text{csqn}}\sum_{JT}\hat{J}\hat{T}\langle ijJT|V|ijJT\rangle. \tag{75}$$

The factor $\frac{1}{2}$ comes from independently summing over i and j rather than the restricted summation $i<j$. The limit csqn refers to summing only over the closed shell quantum numbers (n,l,j). Thus, no m sum is done here; it has already been done. For ^{6}Li, the only closed shell is the $S_{1/2}$ shell. The interaction of a single nucleon with closed shell of other nucleons can be written as

$$A_{CO}(j)=\frac{1}{2\hat{j}}\sum_{i}^{\text{csqn}}\sum_{JT}\hat{J}\hat{T}\langle ijJT|V|ijJT\rangle. \tag{76}$$

In terms of these quantities, we now express the potential energy matrix element for all sets of a' and a. All these contribute to the $J=1$, $T=0$ ground state of ^{6}Li. Whether or not a particular configuration contributes to a given state has been indicated in Table I. We have

$$W^{JT}_{33}=A_{CC}+2A_{CO}(\tfrac{3}{2}^-)+\langle\tfrac{3}{2}^-\tfrac{3}{2}^-JT|V|\tfrac{3}{2}^-\tfrac{3}{2}^-JT\rangle. \tag{77}$$

The factor of 2 is because of the two $P_{3/2}$ nucleons present in this configuration. We also have

$$W^{JT}_{11}=A_{CC}+2A_{CO}(\tfrac{1}{2}^-)+\langle\tfrac{1}{2}^-\tfrac{1}{2}^-JT|V|\tfrac{1}{2}^-\tfrac{1}{2}^-JT\rangle, \tag{78}$$

and

$$W^{JT}_{22}=A_{CC}+A_{CO}(\tfrac{3}{2}^-)+A_{CO}(\tfrac{1}{2}^-)$$
$$+\langle\tfrac{3}{2}^-\tfrac{1}{2}^-JT|V|\tfrac{3}{2}^-\tfrac{1}{2}^-JT\rangle. \tag{79}$$

For the nondiagonal matrix elements we obtain

$$W^{JT}_{32}=\langle\tfrac{3}{2}^-\tfrac{3}{2}^-JT|V|\tfrac{3}{2}^-\tfrac{1}{2}^-JT\rangle, \tag{80}$$
$$W^{JT}_{31}=\langle\tfrac{3}{2}^-\tfrac{3}{2}^-JT|V|\tfrac{1}{2}^-\tfrac{1}{2}^-JT\rangle, \tag{81}$$

and

$$W^{JT}_{21}=\langle\tfrac{3}{2}^-\tfrac{1}{2}^-JT|V|\tfrac{1}{2}^-\tfrac{1}{2}^-JT\rangle. \tag{82}$$

These matrix elements are all plotted versus ρ for the dTS Sprung potential in Fig. 1, for the ground state of ^{6}Li. We note the diagonal values of $W^{JT}_{aa'}$ are in general much larger than the nondiagonal matrix elements. A plot of W versus ρ, the hyper-radius, tends to reflect the value of V_{12} vs r_{12}, namely, a short range repulsion, and a long range attraction.

III. NUMERICAL SOLUTION OF THE COUPLED RADIAL EQUATIONS

In $K_{\min}$ approximation we have to solve Eq. (40) which we write as

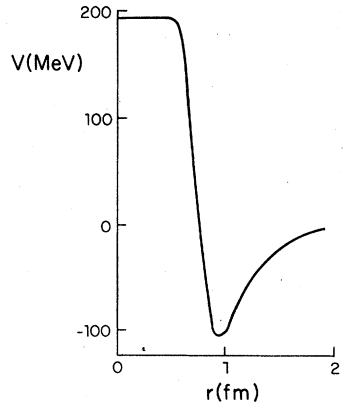

FIG. 1. The dTS central potential (Ref. 23) vs r_{12} for the $S=0$, $T=1$ two-nucleon channel.

$$D\chi_a(\rho) \equiv \left(\frac{d^2}{d\rho^2} - \frac{\mathcal{L}(\mathcal{L}+1)}{\rho^2} - \frac{2m}{\hbar^2} W_{aa}^{JT}(\rho)\right)\chi_a(\rho)$$

$$= B\chi_a + \sum_{a' \neq a} \frac{2m}{\hbar^2} W_{ac}^{JT} \chi_{a'}(\rho) , \qquad (83)$$

where we have defined

$$B = 2m|E|/\hbar^2 . \qquad (84)$$

The boundary conditions to be applied are that $\chi(\rho)$ goes to 0, as ρ approaches 0 or ∞. We assume the $W_{aa'}^{JT}(\rho)$ to be known functions of ρ.

We solve these coupled differential equations by a finite difference iterative technique. We first solve a set of uncoupled equations for F^0 and E_a^0:

$$DF_a^0(\rho) = \frac{2m}{\hbar^2} E_a^0 F_a^0(\rho) , \qquad (85)$$

for each value of a using a finite difference approximation for $d^2F^0/d\rho^2$ where the finite difference is 0.5 fm. Reducing this value by a factor of 2 made no detectable difference in the final calculated energy. The applied boundary conditions are that

$$F_a^0(\rho) \to h_{\mathcal{L}}\left[i\left(\frac{2m}{\hbar^2}E_a^0\rho^2\right)^{1/2}\right] \text{ for large } \rho , \qquad (86)$$

and that F = zero, for ρ equal to two differences (1 fm) less than the value for which the angular momentum barrier exceeds the potential energy matrix element, that is, when

$$\frac{\hbar^2\mathcal{L}(\mathcal{L}+1)}{2m\rho^2} > W_{aa}^{JT}(\rho) . \qquad (87)$$

For small ρ, the angular momentum barrier overwhelms the potential energy matrix element. One loses about two digits of accuracy in the calculation of F for every finite difference step one takes as you approach the origin, in the classically forbidden region. The exact wave function must be very small throughout the forbidden region because $\mathcal{L} = 8$, and the potentials used become repulsive for small hyper-radial values. The calculated binding energies were insensitive to applying the boundary condition

$$F(0) = 0 , \qquad (88)$$

at the origin, or one, two, or three steps inside the classically forbidden region. Thus they were applied at two steps inside the classically forbidden region. That is, rather than Eq. (88), we require

$$F_a^0(1.5) = 0 \qquad (89)$$

as a condition to determine the binding energies E_a^0. Then for ρ less than 2 fm we set

$$F^0(\rho) = (\rho/2)^{\mathcal{L}} F^0(2) . \qquad (90)$$

We normalize for all a, to the condition

$$\int_0^\infty F_a^2(\rho)d\rho = 1 . \qquad (91)$$

We now obtain our first approximation to χ_a by setting approximately

$$\chi_a^0(\rho) \approx R_a^0(\rho) = C_a^0 F_a^0(\rho) , \qquad (92)$$

where the C_a^0 are unknown coefficients we now determine. We first calculate

$$\int F_a^0 D R_a^0 d\rho = B^0 \int F_a^0 R_a^0 d\rho + \sum_{a' \neq a} \frac{2m}{\hbar^2} \int F_a^0 W_{aa'}^{JT} R_{a'}^0 d\rho , \qquad (93)$$

where D is given by Eq. (83). Then we can write

$$\frac{2m}{\hbar^2} E_a^0 C_a^0 = B^0 C_a + \sum_{a' \neq a} C_{a'}^0 V_{aa'} , \qquad (94)$$

where

$$V_{aa'} = \frac{2m}{\hbar^2} \int_0^\infty F_a^0(\rho) W_{aa'}^{JT}(\rho) F_a^0(\rho) d\rho , \qquad (95)$$

and also

$$\sum_a (C_a^0)^2 = 1 . \qquad (96)$$

Equations (94) and (96) provide $a+1$ equations for the $a+1$ unknowns, C_a^0 and B^0, the next estimate for the binding energy. There are a solutions to these equations and a corresponding set of coefficients C_a^0 for each eigenenergy. We take the lowest eigenenergy and its corresponding set of coefficients in general when solving for the ground state, and we now call this set C_a^0. This process is iterated, now using F_a^0 that asymptotically go as $h_{\mathcal{L}}(iB^0\rho)$ for large ρ until convergence is achieved, usually only two iterations. Then we use the coefficients C_a^0 to now solve the equation

$$DF_a^1 = \frac{2m}{\hbar^2} E_a^1 F_a^1 + \sum_{a' \neq a} \frac{2m}{\hbar^2} W_{aa'}^{JT} R_{a'}^0 , \qquad (97)$$

where asymptotically, for large ρ, we take

$$F_a^1(\rho) = C_a^0 F_a^0(\rho) . \qquad (98)$$

These equations we solve (for each a value) for E_a^1 and for F_a^1 by choosing E_a^1 so that F_a^1 vanishes at the origin. Now we calculate the normalization

$$\int_0^\infty [F_a^1(\rho)]^2 d\rho = N_a^2 , \qquad (99)$$

and note that N_a is not necessarily equal to unity. We now use the positive square root of Eq. (99) and take as our next approximation to $\chi_a(\rho)$,

TABLE II. Wave function normalizations from a state dependent potential.

J	T	Binding calculated	Binding experimental	Strength factor	C_3	C_2	C_1
1	1	22.1	15.205[a]	0.928	0.0	1	0.0
1	0	29.11	25.30	0.980	0.045	0.743	0.668
2	1	31.41	25.63	0.952	−0.688	0.725	0.0
2	0	28.90	26.70	0.979	0.0	1	0.0
0	1	38.20	27.44	0.905	0.827	0.0	0.562
3	0	29.05	28.815	0.995	1	0.0	0.0
1	0	31.775	31.0	0.990	0.623	0.507	−0.595

[a] Determined from ^{3}He and ^{3}H binding energies, neglecting Coulomb effects.

$$\chi_a(\rho) \approx R_a^1(\rho) = C_a^1 F_a^1 / N_a \,, \tag{100}$$

where the C_a^1 are unknown constants. They must satisfy

$$\sum_a (C_a^1)^2 = 1 \,.$$

Equations (93)–(96) are reevaluated using R_a^1 and F_a^1 rather than R_a^0 and F_a^0. As a result new values of C_a^1 and B^1 are obtained. Thus the process iterates.[29] The process converges to a solution in about three iterations for the potentials we utilize. Convergence is obtained in the sense that $B^{i+1} = B^i$ to four significant digits, and that $C_a^{i+1} = C_a^i$ to about three digits.

IV. RESULTS: EIGENFUNCTIONS, EIGENVALUES, AND STATE DEPENDENT POTENTIALS

Using the dTS potential,[23] the spectrum of seven ^{6}Li bound states calculated in $K_{\min}$ approximation is shown in Table II. In contrast there are six states seen experimentally. In general the $T = 1$ states are too tightly bound when compared to experiment. The ground state calculated is a $JT = 0, 1$ state, whereas experimentally this state is the second excited state of ^{6}Li. If a slight state dependence to the potential is introduced via an arbitrary strength parameter into the calculated potential energy matrix elements, $W_{ka}^{ka'}$, then one can obtain agreement with the experimental spectrum. If the potential energy matrix elements are

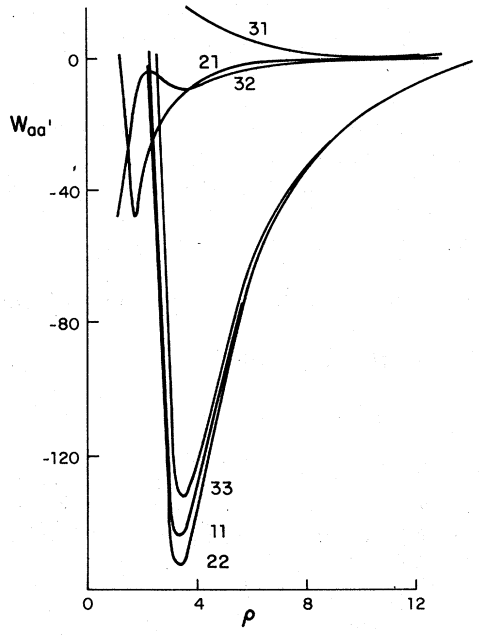

FIG. 2. The hyperspherical potential energy matrix elements $W_{aa'}$ for the ground state of ^{6}Li using dTS soft core potential, in MeV vs the hyperspherical radius ρ in fm. The values of a, a' are labeled on each curve.

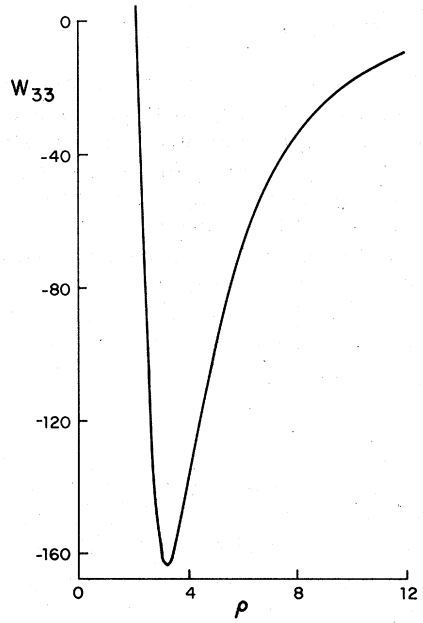

FIG. 3. The hyperspherical potential energy matrix elements W_{33} for the $J, T = 3^+, 0$ states of ^{6}Li using a dTS soft core potential.

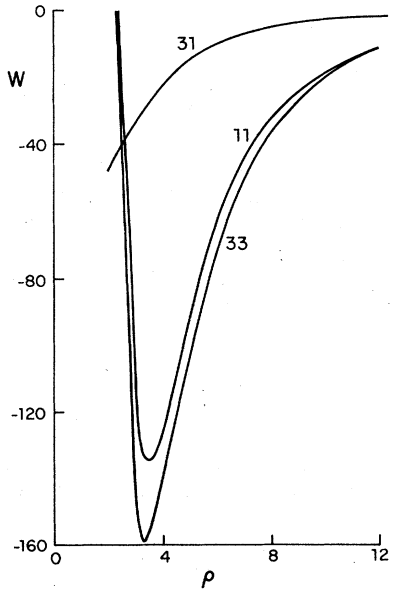

FIG. 4. The hyperspherical potential energy matrix elements $W_{aa'}$ for the J, $T=0$, 1 state of ^{6}Li. The values of a,a' are labeled on each curve.

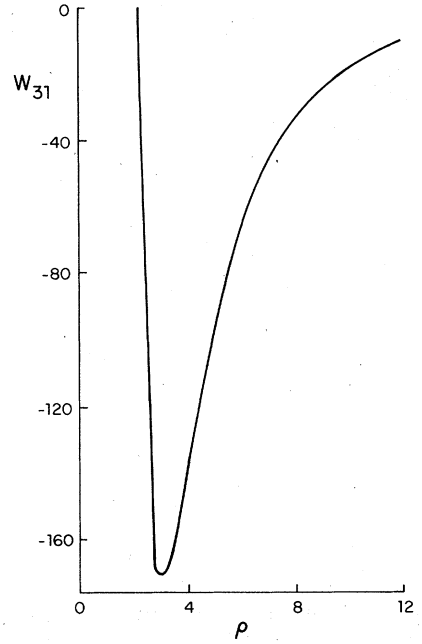

FIG. 6. The hyperspherical potential energy matrix element W_{22} for the $J, T=2$, 0 state of ^{6}Li using dTS soft core potential.

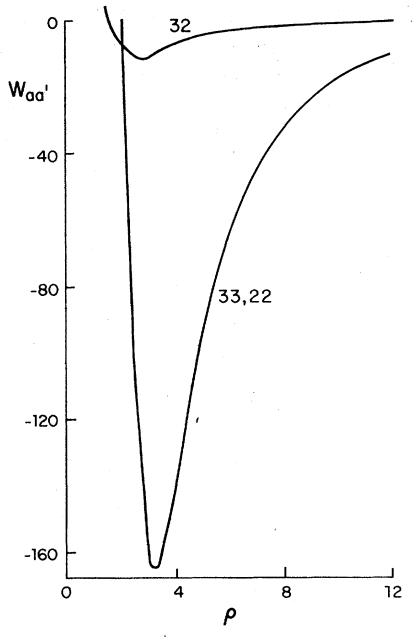

FIG. 5. The hyperspherical potential energy matrix element $W_{aa'}$ for the J, $T=2$, 1 state of ^{6}Li using a dTS soft core potential. The values of a,a' are labeled on each curve.

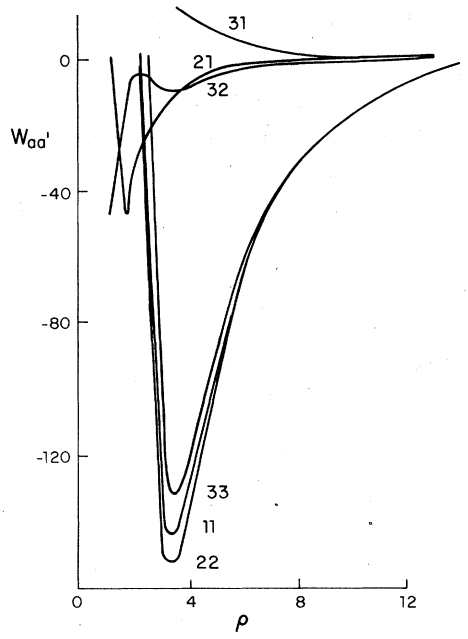

FIG. 7. The hyperspherical potential energy matrix element $W_{aa'}$ for the excited J, $T=1$, 0 state of ^{6}Li using a dTS soft core potential. The values of a,a' are labeled on each curve.

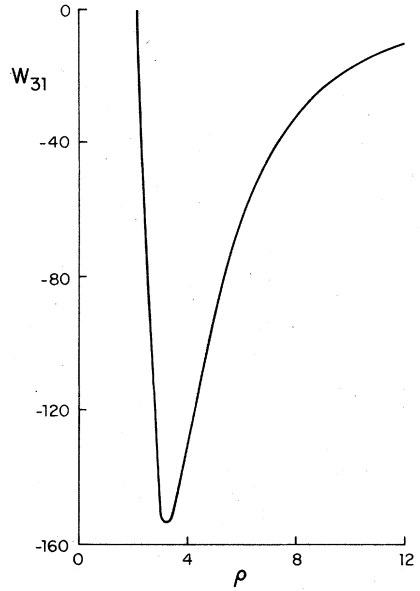

FIG. 8. The hyperspherical potential energy matrix element W_{22} for the J, $T = 1$, 1 state of ^{6}Li using a dTS soft core potential.

multiplied by a state dependent factor ranging from 0.905 to 0.995, then the experimental spectrum is reproduced. These factors are also listed in Table II. The $T = 0$ factor required is practically unity, namely about 0.99, indicating that no change in the potential is needed for these states. For the $T = 1$ states, the factor is 0.905 and 0.952, which averages to 0.928. Thus the $T = 0$ states are calculated to have binding energies that are nearly equal to the experimental values while the $T = 1$ states are 5–10 MeV too tightly bound. This

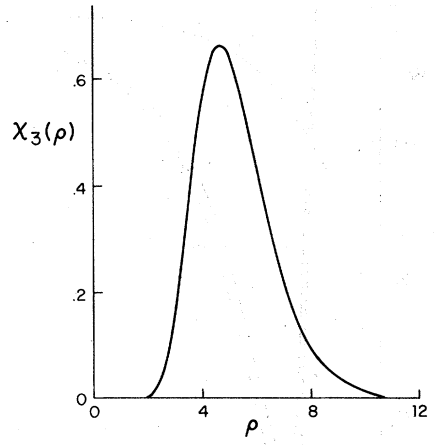

FIG. 10. Hyper-radial wave functions $\chi_3(\rho)$ for the J, $T = 3$, 0 first excited state of ^{6}Li vs the hyper-radius ρ.

isospin difference may reflect the use of the dTS potential. This lack of agreement may partly be due to the neglect of the Coulomb potential. This discrepancy may also be due to the neglect of configurations with K greater than K_{min}. The coupling of the K_{min} configurations to the higher K configurations may well be state dependent. This state dependence may be what the arbitrary state dependent factor is reflecting. Using a factor of 0.928, the $JT = 1^+, 1$ state is calculated to have a binding energy of 15.245 MeV. Such a binding energy is approximately the sum of the Triton and the ^{3}He binding energies. Therefore, we speculate this state may correspond to a nuclear molecule. A "molecule" composed of a

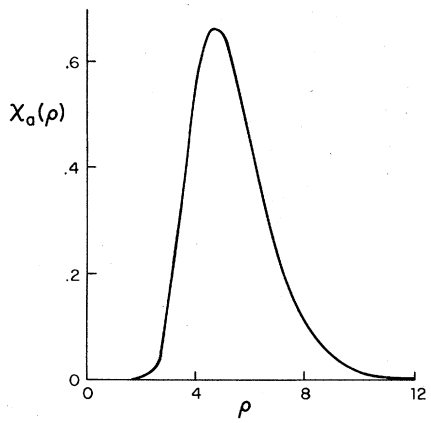

FIG. 9. Hyper-radial wave functions $\chi_a(\rho)$ for the J, $T = 1$, 0 ground state of ^{6}Li vs the hyper-radius ρ. The value of a is labeled on each curve.

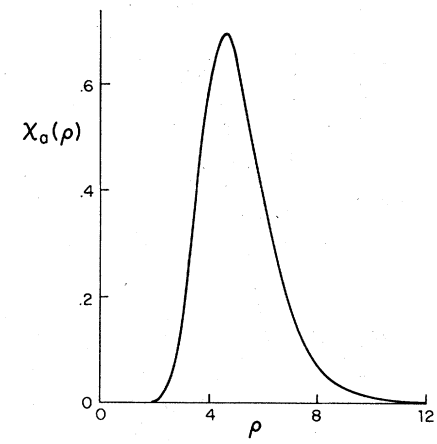

FIG. 11. Hyper-radial wave functions $\chi_a(\rho)$ for the J, $T = 0$, 1 excited state of ^{6}Li vs the hyper-radius ρ. The difference between the two curves is less than the line width used. The value of a is labeled on each curve.

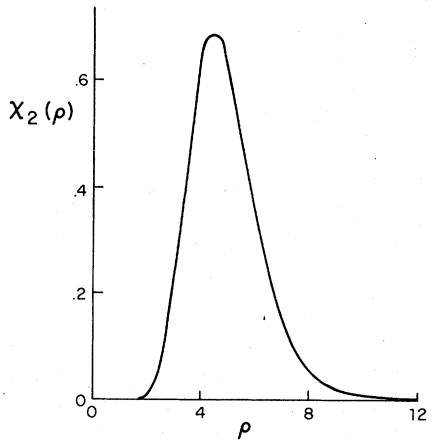

FIG. 12. Hyper-radial wave functions $\chi_2(\rho)$ for the J, $T=2$, 0 excited state of ^{6}Li using dTS soft core potential.

triton and a ^{3}He pair of nuclei could have ground state quantum numbers of $J=0$ or 1, and $T=0$ or 1. This $K_{\min}$ calculation suggests that $JT=1^+,1$.

If the two-nucleon potential were a harmonic oscillator potential, the K harmonics expansion would uncouple in K. Therefore, the coupling potentials between harmonics of different K are connected to the deviation of the two-nucleon potential from a harmonic oscillator potential. It is the hyper-radial angular momentum barrier that brings about convergence to the K harmonic expansion. $K_{\min+1}$ configurations are excluded from consideration for parity reasons. For a $K_{\min+2}$ configuration, the angular momentum barrier becomes $110\hbar^2/2m\rho^2$, instead of $72\hbar^2/2m\rho^2$, for a $K_{\min}$ configuration. For all the bound states, the hyper-radial wave functions had a calculated peak at about 5 fm, and they rapidly go to zero for larger hyper-radius. At $\rho=5$ fm, this is an increase of about 30 MeV in the angular momentum barrier for $K_{\min+2}$ configurations. Thus we believe the $K_{\min}$ configuration is the most important configuration. Its dominance can be determined only by a calculation including $K_{\min+2}$ configurations, however.

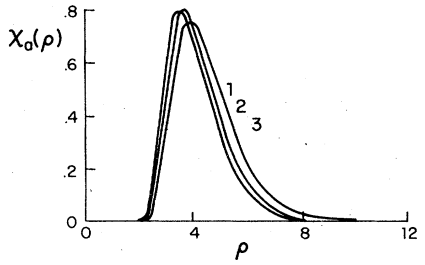

FIG. 14. Hyper-radial wave functions $\chi_a(\rho)$ for the J, $T=1$, 0 excited state of ^{6}Li. The value of a is labeled on each curve.

Having introduced one parameter to the dTS potential, we have an *ad hoc* potential that we are using, although the modification is not very severe from the potential found to fit scattering phase shifts. We present in Table II the strength parameters used to fit the various bound states of ^{6}Li. The fit has a slight state dependence but only a slight one. The fit to the experimental binding is, of course, excellent, as we have varied the potential to fit it, but the variation is small. The $J=1$, $T=0$ excited state was found using the same potentials as were used to fit the ground state. The only difference, compared to finding the ground state, is that the second lowest energy and its corresponding set of coefficients C_a, see Eqs. (93)–(96), were used in iteratively solving the set of coupled differential equations for the

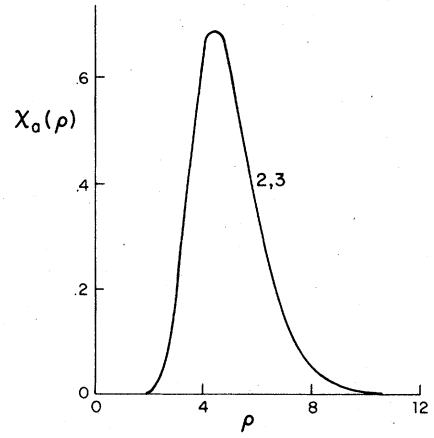

FIG. 13. Hyper-radial wave functions $\chi_a(\rho)$ for the J, $T=2$, 1 excited state of ^{6}Li vs hyper-radius ρ. The difference between the two wave functions is less than the line width used.

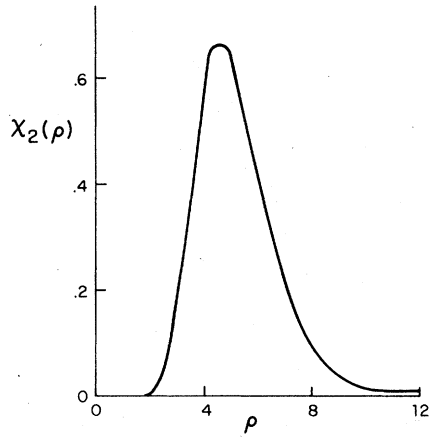

FIG. 15. Hyper-radial wave function $\chi_2(\rho)$ for the predicted J, $T=1$, 1 excited state of ^{6}Li.

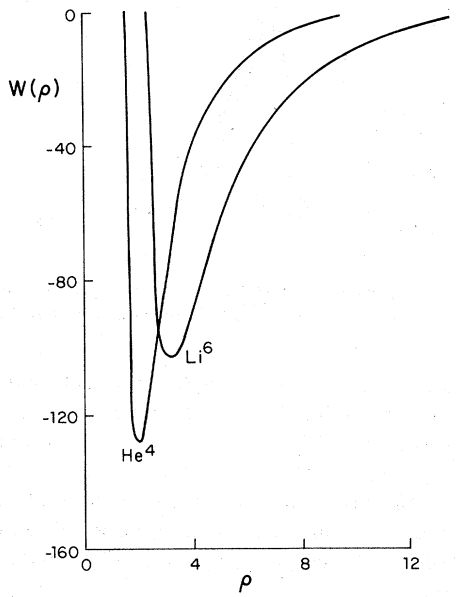

FIG. 16. The $(S_{1/2})^4$ configuration matrix element of the potential energy for the dTS potential, for ^{4}He, and for ^{6}Li, versus the hyper-radius ρ.

binding energy and for the wave functions.

The dTS super-soft-core potential[23] is shown in Fig. 1 for the $S=0$, $T=1$ state vs r_{12}. The super-soft-core terminology means the potential is finite, even at the origin, in contrast to a soft core, which goes as a Yukawa potential at the origin, or in contrast to a hard core potential, which goes to infinity at some nonzero radius.

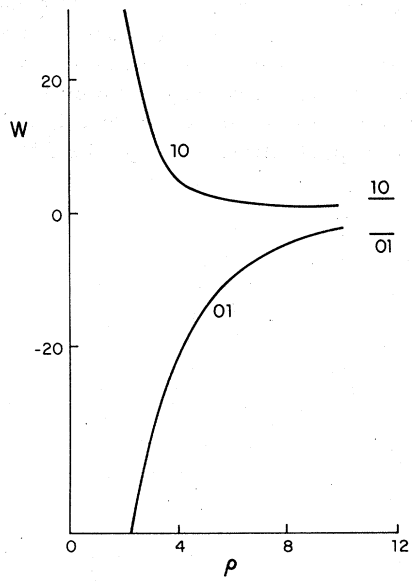

FIG. 17. The $(P_{3/2})^2$, $(P_{1/2})^2$ hyperspherical matrix element of the two nucleon interaction for the various labeled J, T states vs the hyper-radius ρ. The dTS potential is used for the interaction. The bare Sussex values are indicated by a short line on the right side.

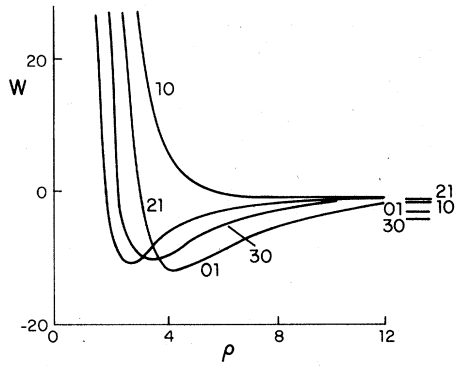

FIG . 18. The two-nucleon $(P_{3/2})^2$, $(P_{3/2})^2$ hyperspherical matrix element of the two-nucleon interaction for various labeled J, T states vs the hyper-radius ρ. The bare Sussex values are indicated by a short line on the right side.

The matrix elements for the unmodified dTS potential are shown in Figs. 2–8. The calculated eigenfunctions for the corresponding states are shown in Figs. 9–15. The coefficients C_a are listed in Table II.

We now compare the potential energy matrix elements of the original dTS potential. The matrix elements become positive at about 2 fm and for smaller hyper-radial values as well. The minimum in the diagonal potential energy matrix elements vs the hyper-radius, is at about 4 fm. The matrix element for large hyper-radius goes approximately as ρ^{-3}.

The nondiagonal matrix elements are small compared to the diagonal matrix elements for the dTS potential for all the states of ^{6}Li. This small relative size aids the convergence of the solution to the coupled equations. Since the nondiagonal

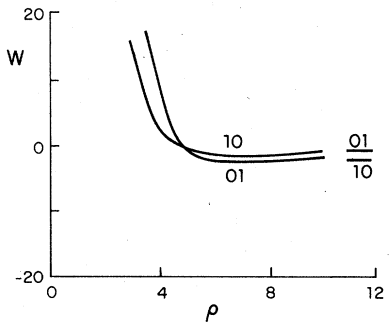

FIG. 19. The two-nucleon $(P_{1/2})^2$, $(P_{1/2})^2$ hyperspherical matrix element vs ρ, for various labeled J, T values. The bare Sussex values are indicated by a short line on the right side.

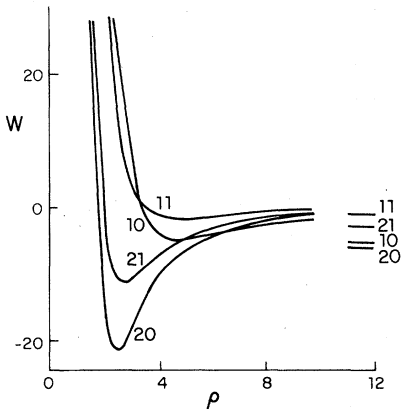

FIG. 20. The two-nucleon $(P_{3/2}P_{1/2})$, $P_{3/2}P_{1/2}$ hyperspherical matrix element vs ρ, for various labeled J, T values. The bare Sussex values are indicated by a short line on the right side.

matrix elements are small, their initial neglect is not too drastic in obtaining the first approximate solution of the coupled equations. It is the nondiagonal matrix elements that provided the coupling to the differential equations. Shown in Figs. 3–8 are the potential energy matrix elements for the other excited states of ^{6}Li. In every instance the nondiagonal matrix elements are much smaller than the diagonal matrix elements. The ratio might be characterized as approximately 1:36, that is 1 to N squared. The lowest energy solutions to the coupled differential equations are all nodeless, that is, they vanish only at zero and infinite values of the hyper-radius. The solutions have a single peak at about 5 fm, located approximately where the diagonal matrix element plus the angular momentum barrier combined have their minimum value.

The coefficients C_a, when squared are the probability that a given configuration a, is present

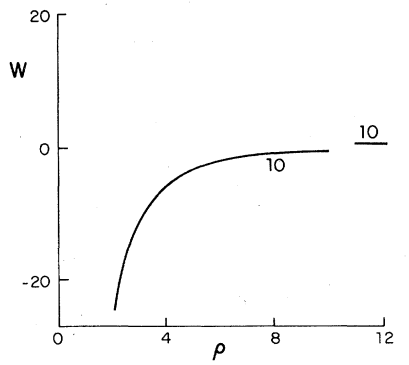

FIG. 21. The two-nucleon $(P_{3/2}P_{1/2})$, $(P_{1/2})^2$ hyperspherical matrix element vs ρ, for various labeled J, T values. The bare Sussex values are indicated by a short line on the right side.

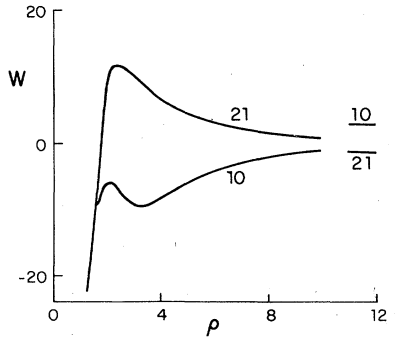

FIG. 22. The two-nucleon $(P_{3/2}P_{1/2})$, $(P_{3/2})^2$ hyperspherical matrix element vs ρ, for various labeled J, T values. The bare Sussex values are indicated by a short line on the right side.

in a given wave function. All the wave functions plotted as $\chi_a(\rho)$ are normalized to unity.

The coefficients C_a are similar to certain coefficients in the shell model. In a configuration interaction calculation within the harmonic oscillator shell model with several configurations, the probability of a given configuration is found from a variational calculation. Thus, this sort of calculation is analagous to assuming the hyper-radial functions are

$$C_a\chi(\rho) = C_a\delta(\rho - \rho_0)\,,$$

where ρ_0 is related to the harmonic oscillator radius via Eq. (60), and C_a would be determined by minimizing the energy. We note the hyper-radial functions calculated are not δ function in shape, but there is a resemblance in that they are a function with a single peak and decrease monotonically on either side of that peak. The half width as half maximum is on the order of 1 fm. The values of the C_a reported in Table II reflect an attractive spin orbit two nucleon potential as C_3 is larger than C_1 in magnitude, for the ground state of any set of J, T values. For excited states with a given J, T, the reverse is true.

The electromagnetic form factors for ^{6}Li are not calculated here as that seems difficult[15,22,30] enough to merit a separate study. We note, however, that the expectation value of ρ^2 for the ground state wave function is 28.86 fm^2. This implies an rms charge radius of 2.2 fm, which is less than the experimental[31] charge radius of 2.56 fm for ^{6}Li. This calculated value assumed the protons were distributed the same as were the neutrons and also assumed that the protons were point charges. The relaxation of both these assumptions would tend to increase the calculated charge radius. Nonetheless, we are not surprised at calculating too small a rms charge radius for ^{6}Li, because the dTS potential used is a very-

soft-core potential, and the wave function used slightly overbinds ^{6}Li. This shifts the wave function to smaller values of ρ and results in the calculated expectation value of ρ^2 being too small. A J, $T=1,1$ state is calculated with a binding energy of 15.245 MeV. From this binding energy it appears similar to a ^{3}H ^{3}He nuclear molecule. No experimental evidence of such a state appears to exist.[8]

V. CONTRASTS WITH OTHER MODELS

A. Core polarization

If one considered the ^{4}He ground state to be simply a $S_{1/2}{}^4$ configuration of two neutrons and two protons, the appropriate potential matrix element for the ^{4}He ground state would be given by the quantity named A_{CC} in Eq. (75). In Fig. 16, we plot the $S_{1/2}{}^4$ configuration matrix element of the potential energy for the dTS potential. We plot this matrix element for the dTS two nucleon potential. We show the result for both ^{4}He and also a plot of the same potential energy matrix element for the $S_{1/2}{}^4$ configuration of nucleons within ^{6}Li. The two curves are different. This difference we call core polarization, somewhat in analogy to the term commonly used in reaction theory. The two calculated curves are based on the exact same two-nucleon potential. The two calculated curves are different because the matrix element, see Eq. (58), depends on the number of nucleons present. This difference is neglected in models of ^{6}Li that treat this nucleus as an α, a neutron, and a proton. These models sometimes attempt to account for this effect by using "effective potentials" rather than real potentials. This difference also effects the interpretation of experimental binding energies being related to the interaction of the outside nucleons as calculated by

$$B(np) = B(^6\mathrm{Li}) - B(^4\mathrm{He}) - [B(^5\mathrm{Li}) - B(^4\mathrm{He})]$$
$$- [B(^5\mathrm{He}) - B(^4\mathrm{He})]$$
$$= -6.62 \text{ MeV}.$$

This difference is also neglected in three body models of ^{6}Li that assume the α in the ^{6}Li is the same as an isolated ^{4}He nucleus.

This K harmonics solution of the six nucleon problem does not assume the interaction matrix element of the four nucleons forming a prototype α particle is the same as in ^{6}Li as it is in ^{4}He. We see for the dTS potential this difference is not negligible and should be incorporated in other calculations, if it were possible to do so.

Using a $K_{\min}$ formulation for ^{4}He, we calculate a ^{4}He binding energy of 29.3 MeV. Combining this with the calculated ^{6}Li $JT = 1^+0$ binding energy of 31.775 MeV, we calculate a ^{6}Li that is stable to α plus deuteron decay.

B. Shell model effective interactions

In the shell model calculations, one problem is the choice of effective "residual two-body" interactions that is appropriate to use for the chosen configuration space. By making reasonable assumptions about the smoothness and range of the two nucleon potential, Elliot and his co-workers[31,32] at Sussex were able to deduce the relative harmonic oscillator matrix elements directly from the phase shifts. So called bare matrix elements were calculated, as well as various corrections to their interaction matrix element via degenerate perturbation theory.[19,33] In Figs. 17–22 we indicate their tabulated bare matrix elements obtained[17] using an oscillator length parameter $b = 1.7$ fm. Incorporating the various shell model configuration corrections[17] never changed the sign of the bare matrix element obtained and resulted in a magnitude change typically of 20%. We, therefore, compare the bare matrix elements to the corresponding hyperharmonic nondiagonal matrix elements, see Eq. (80)–(82). These are not identical quantities to compare, in part because the derivation of the effective interaction is one of the basic problems of the shell model.[19] The hyperharmonic method, though, does offer a natural way to obtain an analogous quantity, namely, the nondiagonal matrix element of the potential energy is equivalent to the shell model matrix element of the "effective interaction." We note the hyperharmonic nondiagonal matrix element is a function of the hyperradius, ρ, and is so plotted in Figs. 17–22. At what value of ρ should the comparison be made? If the hyperharmonic matrix elements were evaluated using the saddle point or method of steepest descent, we would have

$$\rho[K + \tfrac{3}{2}(N-1)]^{1/2} b = (2 + \tfrac{19}{2})^{1/2} 1.7$$
$$= (\tfrac{19}{2})^{1/2} 1.7 \approx 5 \text{ fm}.$$

On the other hand, the most characteristic hyperradial value may be the one that maximizes the hyper-radial wave function $\chi_a(\rho)$. This is seen to be typically 5–5.5 fm (see Figs. 9–15). The nondiagonal matrix element of the hyperspherical method is evaluated using the dTS potential as this provides an excellent fit to the two nucleon scattering data and should be most nearly comparable to the bare matrix evaluated. Inspection of the curves shows that agreement between the

two calculations is approximate only. For the $\langle (P_{1/2})^2|V|(P_{3/2})^2\rangle$ matrix element, the two methods agree for a ρ of 8, if $J, T = 0$, and for ρ equals 5.0 for $J, T = 1, 0$. Perhaps a more realistic test would be to calculate the integral

$$\int \chi_a W^{JT}_{aa'} \chi_{a'} d\rho$$

and compare this weighted integral with the Sussex calculation. Doing the integral results in integrated values comparable in magnitude and of the same sign as the Sussex matrix elements for this case. Such cannot be said for all the other cases. However, for the $\langle (P_{3/2})^2|V|(P_{3/2})^2\rangle$ matrix element, the $J, T = 1, 0$ hyperharmonic calculated matrix element is generally too repulsive (positive) compared to the other J, T values, but the general trend of the Sussex matrix elements is reproduced. For the $\langle (P_{1/2})^2|V|(P_{1/2})^2\rangle$ matrix element, the calculated $J, T = 0, 1$ matches the Sussex value quite well, but the $J, T = 1, 0$ value is again too repulsive compared to the Sussex value. For the $\langle P_{3/2}P_{1/2}|V|P_{3/2}P_{1/2}\rangle$ matrix element, the calculated values tend to reproduce the trends of the Sussex values. However, the $J, T = 2, 1$ state is calculated as too attractive compared to the Sussex value. For the $\langle P_{3/2}P_{1/2}|V|(P_{1/2})^2\rangle$ matrix element, with $J, T = 1, 0$, the calculated matrix value is attractive, but the Sussex value has the opposite sign. Finally, for the $\langle (P_{3/2})^2|V|P_{3/2}P_{1/2}\rangle$ matrix element, the calculated values show little hint of possible agreement with the Sussex values. For $J, T = 1, 0$ the calculated value is negative, while the Sussex value is positive. For the $J, T = 2, 1$ case, the calculated matrix element is generally positive, while the Sussex value is negative.

We have been comparing two calculations here. There is a general sense of agreement between them, but the detailed comparison shows differences, in some cases, differences of sign. It is possible that a potential oscillating about "the correct potential" could reproduce scattering phase shifts well and still fail to agree with the Sussex matrix element. We are comparing small bits and pieces of the potential here in a detailed manner. Secondly, the two quantities being compared would not match exactly, even if an identical two-body potential were used in both, due to the differing treatment of the geometry with respect to the center of mass motion. The Sussex treatment tries to avoid a potential. Anyway, we have here a prescription of obtaining effective interaction for shell model calculations working directly from a two-nucleon potential, without a hard core. One simply evaluates the nondiagonal matrix element of the potential energy in the hypersphere formalism at a value of $\rho = [K + 3/2(N-1)]^{1/2} b$, where b is the oscillator length parameter.

Other improvements of this prescription can be found, possible, but even this first prescription offers a guide to obtaining an effective interaction for shell model calculations.

C. Convergence of the hyperspherical harmonic solution to Li^6

One must go beyond $K_{\min}$ calculations to test the convergence of the method. That has not been done here. The three-nucleon problem did not converge[3,2] at $K = K_{\min}$, but instead harmonics out to about $K = 7$ were found to contribute. For N greater than four, only one calculation has used K greater than $K_{\min}$, the $K_{\min+2}$ calculation of Sadovoi and Siminov[6] for the ^{16}O ground state. They found the contribution of $K_{\min+2}$ harmonics to the binding energy to be about 25% in a "model calculation" and that single particle excitations where n increased rather than the orbital angular momentum l increases were the most important. The brunt of their calculation suggests that K greater than $K_{\min}$ should be investigated for ^6Li. This will be reported on in a subsequent work. The agreement between the calculated spectrum and the experimental spectrum offers another reason for believing the influence of $K_{\min}$ configurations is dominant. Experiment shows that odd parity states are more than 20 MeV excited in energy. These would correspond to $K_{\min+2}$ configurations can be expected then at about 40 MeV of excitation. No states capable of being produced by a $K_{\min+2}$ configuration, and not by a $K_{\min}$ configuration, such as a 4^+ or a 5^+ are seen in the experimental spectrum.

VI. SUMMARY

We have presented a systematic way of solving the six-nucleon bound state problem. Only soft core potentials can be used in the hyperspherical method. The center of mass motion has been removed from the usual nonrelativistic N-body Schrödinger equation. Slater determinants are used to construct antisymmetric hyperharmonic polynomials of definite J, J_z, T, and T_z. A set of coupled one dimensional radial equations are obtained from the Schrödinger equation when the N-body wave function is expanded as

$$\psi(1, 2, \ldots, N) = \frac{1}{\rho^{(3N-4)/2}} \sum_{ka} \chi_{ka}(\rho) Y_{ka}(\Omega) .$$

The summation over K is truncated at its minimal value consistent with the antisymmetrization requirement. A many-body angular momentum barrier tends to justify this truncation. A po-

tential with phase shift credentials is used, and results in calculated binding energies in fair agreement with experiment. A modified potential that is slightly state dependent could be used to bring about agreement with experimental binding energies. The *dTS* potential used has central, tensor, spin orbit, and L squared parts.[23] Each part resembles a sum of meson exchange contributions and has soft, finite, repulsive core. The numerical solution to the coupled radial equations are shown and compared to the shell model. The proper handling of the potential energy matrix element with center of mass motion excluded is detailed. A prescription for obtaining effective interactions for shell model type calculations is presented. The results of this prescription are compared to the bare Sussex matrix elements. The agreement is fair.

The difference in the potential energy matrix element of four $S_{1/2}$ nucleons in a ^{4}He nucleus or in a ^{6}Li nucleus is shown not to be zero. A $J,T = 1,1$ state is found with a binding energy of 15.245 MeV. This binding energy spin, parity, and isospin suggests the state may resemble a nuclear molecule of ^{3}H and ^{3}He. Further work is suggested along the lines of a $K_{\min+2}$ calculation.

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