Relationship between effective and realistic interactions in ^{6}Li

Paul Goldhammer
Department of Physics and Astronomy, University of Kansas, Lawrence, Kansas 66045
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A variational trial wave function is used to develop a perturbation expansion for the effective shell model interaction in the case of a degenerate zero-order basis. The form of this trial function is suggested by the Brillouin-Wigner perturbation procedure, and the Moszkowski-Scott separation method. Application is made to the low lying levels of ^{6}Li. The absolute binding energies obtained are 4 to 5 MeV short of experimental values. Acceptable agreement with experiment is found for the energy level spacing.

I. INTRODUCTION

The usual assumption made in applications of the nuclear shell model[1,2] (SM) is that one may employ a Hamiltonian composed of one- and two-body operators

$$H_{\rm SM}=\sum_i H_0(i)+\sum_{i<j} v_{ij} \tag{1}$$

in a truncated basis of single particle states. For nuclei in the mass range $5\le A\le 16$, for example, one considers only the states provided by the $(0s)^4(0p)^{A-4}$ particle configuration, with constant single particle energies and two-body matrix elements throughout the shell.

The success of this simple procedure has been most remarkable, despite the fact that realistic nuclear forces are known to be highly singular and must produce significant configuration mixing. The earliest attempts to formally relate the shell model to realistic interactions was in the context of the Brueckner method.[3–5] Block and Horowitz[6] have performed a separation between the energies of the core and valence nucleons, such that the shell model appears to arise naturally out of the perturbation expansion. Brandow[7] later presented a most definitive study of the linked cluster properties of a degenerate perturbation series.

The exact formal solution to the problem is well known.[7] It will be convenient to review it here; in order to compare it with the method presented in Sec. II, and to define some notation. First the Hamiltonian is written as the sum of two terms

$$H=H_0+W\ , \tag{2}$$

where H_0 has known solutions

$$H_0\varphi_n=\epsilon_n\varphi_n\ . \tag{3}$$

Now when one constructs the eigenfunctions ψ_N of H,

$$H\psi_N=E_N\psi_N\ , \tag{4}$$

one selects a certain number of low lying levels in ϕ_n. This may be a degenerate set, or just a "quasidegenerate" subspace lying so close in energy that one expects considerable mixing among them. This is the "model" subspace, and we will designate these states by Latin indices (ϕ_i). States outside the model space will be designated by Greek indices (ϕ_α). One may express the exact wave function by the series

$$\psi_N=\sum_i C_i^N\varphi_i+\sum_\alpha A_\alpha^N\varphi_\alpha\ . \tag{5}$$

Eden and Francis[5] define a model operator:

$$\Omega_N=1+\sum_\alpha \frac{|\alpha\rangle\langle\alpha|}{E_N-H_0}W\Omega_N\ , \tag{6}$$

so that one can write

$$\psi_N=\Omega_N\Phi_N\ , \tag{7}$$

where

$$\Phi_N=\sum_i C_i^N\varphi_i\ , \tag{7a}$$

and we choose to normalize the model space wave function

$$\langle\Phi_N\,|\,\Phi_N\rangle=\sum_i |\,C_i^N\,|^2=1\ . \tag{7b}$$

Algebraic solution to Eqs. (4)—(7) yields the set of relations:

$$(E_N-\epsilon_i)C_i^N=\sum_j\langle\varphi_i\,|\,v_N\,|\,\varphi_j\rangle C_j^N\ , \tag{8}$$

$$E_N=\langle\Phi_N\,|\,H_0+v_N\,|\,\Phi_N\rangle\ , \tag{9}$$

where

$$v_N=W\Omega_N\ . \tag{10}$$

If H_0 is chosen to be a sum of single particle operators $[\sum H_0(i)]$, then clearly v_N will play the role of the shell model effective interaction in the model space (ϕ_i) for Eq. (1). One should note that, in this exact form, the effective interaction is state dependent through the energy denominator in Eq. (6).

Although the solution is formally simple, calculations in the physically interesting examples are clearly not easy. In general one must be content to do approximate summations over α in Eq. (6), to include only certain sets of states or "diagrams."[8,9]

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II. THE VARIATIONAL WAVE FUNCTION

Let us introduce the variational trial wave function

$$\psi_N=\sum_i C_i^N\left[\varphi_i+\sum_{\alpha,n}K_n\frac{\varphi_\alpha\langle\alpha\,|\,W^n\,|\,i\rangle}{E_N-\epsilon_\alpha}\right]. \tag{11}$$

The energy is to be computed starting from

$$E_N=\frac{\langle\psi_N\,|\,H\,|\,\psi_N\rangle}{\langle\psi_N\,|\,\psi_N\rangle}\,, \tag{12}$$

while the C_i^N and K_n are variational parameters to be determined by the conditions

$$\frac{\partial E_N}{\partial C_i^N}=\frac{\partial E_N}{\partial K_n}=0\,. \tag{13}$$

The W^n are a set of potential operators, which are to be chosen through criteria of mathematical convenience and the variational flexibility in the trial function.

Similar trial wave functions have been previously employed in a series of papers.[10,11] It is a natural refinement of the trial function used to generate the Brillouin-Wigner perturbation series.[12,13] Equation (11) merely represents the extension of this function to the case where the zero-order portion of the unperturbed vector space consists of either a degenerate set of functions, or else a set lying too close in energy to rely on perturbation theory to compute the proper admixture of states. Brandow[7] refers to this latter case as a "quasidegeneracy."

Substituting ψ into Eq. (12), and imposing the conditions in Eq. (13) yields:

$$\sum_{i,j}E_2^{ij}(n)C_i^{N*}C_j^N=\sum_{i,j,m}C_i^{N*}C_j^NK_m[E_{ij}^{(3)}(n,m)-E_{ij}^{(2)}(n,m)]\,, \tag{14}$$

$$E_NC_i^N=\sum_jC_j^N\left[\langle i\,|\,H\,|\,j\rangle+\sum_nK_nE_j^{ij}(n)\right], \tag{15}$$

$$E_N=\sum_{i,j}C_i^{N*}C_j^N[\langle i\,|\,H\,|\,j\rangle+K_nE_j^{ij}(n)]\,, \tag{16}$$

where

$$E_2^{ij}(n)=\sum_\alpha\frac{\langle i\,|\,H\,|\,\alpha\rangle\langle\alpha\,|\,W^n\,|\,j\rangle}{E_N-\epsilon_\alpha}\,, \tag{17}$$

$$E_{ij}^{(2)}(n,m)=\sum_\alpha\frac{\langle i\,|\,W^n\,|\,\alpha\rangle\langle\alpha\,|\,W^m\,|\,j\rangle}{E_N-\epsilon_\alpha}\,, \tag{18}$$

$$E_{ij}^{(3)}(n,m)=\sum_{\alpha,\beta}\frac{\langle i\,|\,W^n\,|\,\alpha\rangle\langle\alpha\,|\,W\,|\,\beta\rangle\langle\beta\,|\,W^m\,|\,j\rangle}{(E_N-\epsilon_\alpha)(E_N-\epsilon_\beta)}\,. \tag{19}$$

Equations (15) and (16) have the appearance of a typical matrix eigenvalue problem, and one can easily identify the matrix elements of the shell model Hamiltonian in Eq. (1) as

$$\langle i\,|\,H_{\rm SM}\,|\,j\rangle=\langle i\,|\,H\,|\,j\rangle+\sum_nE_2^{ij}(n)=\left\langle i\left|H_0+W\left[1+\sum_{n,\alpha}K_n\frac{\langle\alpha\rangle\langle\alpha\,|\,W^n}{E_N-\epsilon_\alpha}\right]\right|j\right\rangle. \tag{20}$$

This result should now be compared with the exact solution presented in Sec. I. It is easily seen that the trial wave function in Eq. (11) is equivalent to approximating the model operator of Eden and Francis in the form

$$\Omega_N\rightarrow1+\sum_nK_n\sum_\alpha\frac{|\,\alpha\rangle\langle\alpha\,|\,W^n}{E_N-\epsilon_\alpha}\,, \tag{21}$$

and then determining the K_n to optimize the energy eigenvalue. Physically, one has chosen a variational form of the model operator which is capable of precisely reproducing the effect of all two-body excitations out of the ground state when the W^n are restricted to two-body operators with adequate variational flexibility. The relationship between this procedure and the Brueckner method has been discussed in previous papers.[11]

The eigenvalue problem can be recast into a much more compact form. One may define a column matrix K of the elements K_n, square matrices $E^{(2)}$ and $E^{(3)}$ out of

$$E^{(2)}(n,m)=\sum_{i,j}C_i^{N*}C_j^NE_{ij}^{(2)}(n,m) \tag{22}$$

and

$$E^{(3)}(n,m)=\sum_{i,j}C_i^{N*}C_j^NE_{ij}^{(3)}(n,m)\,. \tag{23}$$

In addition, we need column matrices E_2^{ij} composed of the elements of $E_2^{ij}(n)$, and E_2 out of the elements of

$$E_2(n)=\sum_{i,j}C_i^{N*}C_j^NE_j^{ij}(n)\,. \tag{24}$$

One can now formally eliminate the variational parameters K_n from Eqs. (14)—(16) by matrix algebra to obtain the final relations

$$E_NC_i^N=\sum_jC_j^N[\langle i\,|\,H\,|\,j\rangle+\tilde{E}_2(E^{(3)}-E^{(2)})^{-1}E_2^{ij}]\,, \tag{25}$$

and

$$E_N=\sum_{i,j}C_i^{N*}C_j^N[\langle i\,|\,H\,|\,j\rangle+\tilde{E}_2(E^{(3)}-E^{(2)})^{-1}E_2^{ij}]\,. \tag{26}$$

One must carefully note that the effective shell model interaction

$$\langle i\,|\,H_{\rm SM}\,|\,j\rangle=\langle i\,|\,H\,|\,j\rangle+\tilde{E}_2[E^{(3)}-E^{(2)}]^{-1}E_2^{ij} \tag{27}$$

is now state dependent in two respects. First the matrices E_2^{ij}, $E^{(2)}$, $E^{(3)}$ all appear with the final eigenvalue (E_N) in the energy denominator. This energy dependence has been well documented previously,[7] but in the present work it takes an especially simple form. In the application of this method to nondegenerate systems[11] the Hamiltonian was separated into $H=H_0+W$ in such a way that the energy denominators were held constant while the energy eigenvalue was iterated to self-consistency. This was accomplished through a uniform displacement, U:

$$H_0\rightarrow H_0-U\,, \tag{28a}$$

$$W\rightarrow W+U\,, \tag{28b}$$

which can be varied to redefine unperturbed energies (ϵ_α). The object of this ploy was merely mathematical simplicity. The value of U was iterated in order to hold the energy denominators at a constant value at which many of the integrals in the perturbation series could be performed in closed form. There is also the clear added advantage that each integral only needs to be computed once during the iteration process.

In this procedure the only way the value of U appears explicitly in the perturbation series is in the terms like

$$\sum_{\alpha,\beta} \frac{W^n_{i\alpha} U_{\alpha\beta} W^m_{\beta j}}{(E_N-\epsilon_\alpha)(E_N-\epsilon_\beta)} = U \sum_\alpha \frac{W^n_{i\alpha} W^m_{\alpha j}}{(E_N-\epsilon_\alpha)^2} , \tag{29}$$

which arise in the construction of $E^{(3)}$. Now consider the normalization integral

$$\langle \psi_N \mid \psi_N \rangle = \sum_{i,j} C^{N*}_i C^N_j \left[\delta_{ij} + \sum_{n,m} K^*_n K_m N^{nm}_{ij} \right] , \tag{30}$$

where

$$N^{nm}_{ij} = \sum_\alpha \frac{W^n_{i\alpha} W^m_{\alpha j}}{(E_N-\epsilon_\alpha)} . \tag{31}$$

One now sees that the energy dependence of the effective interaction will depend on the variation of the E_N through a change in $U(\delta U)$ multiplied by the $N_{ij}(n,m)$ (which measure the admixture of states beyond the model space). All this results in a change in the elements of $E^{(3)}$:

$$\delta E^{(3)}_{ij}(n,m) = \delta U N^{nm}_{ij} . \tag{32}$$

It is interesting to estimate this effect. If one suppresses any variation in the C_i for the moment then Eq. (14) will yield a change in the K_m (δK_m) for a small change δU approximated by

$$\begin{aligned} \delta K &\cong -\delta U (E^{(3)}-E^{(2)})^{-1} N K , \\ &\cong -\delta U (E^{(3)}-E^{(2)})^{-1} N (E^{(3)}-E^{(2)})^{-1} E_2 , \end{aligned} \tag{33}$$

where δK is a column matrix formed from the δK_m, and N is a square matrix composed of the elements of

$$N(n,m) = \sum_{i,j} N^{nm}_{ij} C^{N*}_i C^N_j . \tag{34}$$

The variation in the shell model matrix elements is then given as

$$\begin{aligned} \langle i \mid \delta H_{\rm SM} \mid j \rangle \cong -\delta U \tilde{E}_2 (E^{(3)}-E^{(2)})^{-1} N \\ \times (E^{(3)}-E^{(2)})^{-1} E^{ij}_2 . \end{aligned} \tag{35}$$

Comparing Eqs. (27) and (35) we see that the relative size of the change in $H_{\rm SM}$ will depend on the size of the matrix elements of

$$\delta U (E^{(3)}-E^{(2)})^{-1} N . \tag{36}$$

It should be emphasized that Eq. (35) is only intended as a crude estimate of the order of magnitude of this effect, which has been presented for pedagogical purposes. In the actual calculations it is only proper (and actually easier once the programs are written) to solve Eqs. (25) and (26) self-consistently. Results are discussed in Sec. III.

In addition to the energy dependence, the matrix elements of $H_{\rm SM}$ appear to retain a state dependence on the shell model parameters C_i. This effect seems more complex, possibly because it is less familiar. This dependence will cancel out altogether in the absence of coupling between the various two-body channels (represented by the W^n) in the trial wave function. Since channel coupling is rather small with the Paris potential,[14] one might suspect that this effect is not too large.

It is easy to recognize the physical origin of this effect. Consider a specific component (ϕ_i) in the shell model basis. The question is whether the configuration mixing associated with this single vector is independent of the amplitude of the other shell model basis functions. Obviously it will be *only* so long as it is not coupled to these other terms in the perturbation matrices. The effect is also present in the exact formulation of the effective interaction problem. It is concealed, however, within the state dependence of the model operator Ω_N. Assuming a specific trial form for the model operators, as we have done above, clearly brings this dependence forth.

Thus far in this section we have concentrated on the details of the method which arise from the degeneracy in the zero-order wave function. All other details proceed as described in Ref. 11. In particular the operators W^n will be chosen in the form of a projection operator for a specific two-body channel multiplied by a Gaussian radial dependence:

$$W^n(i,j) = P_n(i,j) \exp(-\alpha_n r^2_{ij}) . \tag{37}$$

Individual W^n will be assigned to each two-body channel in the trial wave function, with five radial terms having $\beta_n[\beta_n = \alpha_n/(\alpha_n+1)]$ taking on the values 0.1, 0.3, 0.5, 0.7, and 0.9 in each. This prescription was used previously[11] for the α particle and yielded reasonable results. This procedure was motivated by the Moszkowski-Scott separation method.[15] The method for performing the integrals and making the Pauli correction are precisely as described in Ref. 11.

One note on the Pauli correction is worthwhile. Previous applications of the method have been to the $0s$ shell, where the Pauli principle simply forbids scattering of two nucleons into the same state as in the zero-order wave function. In application to the $0p$ shell one also must forbid terms where two $0p$ nucleons are scattered into the $0s$ shell; or conversely, where two $0s$ nucleons are scattered into the occupied orbitals of the $0p$ shell. Such processes are suppressed automatically through the consistent use of a wave function which is antisymmetric in the exchange of any pair of nucleons. Therefore it is, of course, essential to retain all multiparticle terms in the perturbation series. The mathematical details for making the Pauli correction term proceed as before,[11] just as if this complication was not present.

III. EXAMPLE

The simplest example appropriate to degenerate perturbation theory to be found in nuclear structure is in the low

lying energy levels with $A=6$. In particular, ^{6}Li has six levels with well-established shell model properties.[9,16–18] The interaction used was the Paris potential,[14] which is very easy to work with in this method.[11] The oscillator size parameter was kept at $b=1.6\times10^{-13}$ cm in all calculations.

Results are displayed in Table I. There are three ways to present the data, and comparisons among them are interesting. The first two data columns compare experimental net binding energies with their computed counterpart. The computed energies appear short of experiment by 2 to 3 MeV, but there is another point to be considered. Coulomb interactions were not included in the calculated values, and cannot be deducted from the experimental results in an unambiguous manner. The Coulomb energy in ^{6}Li can be estimated to be somewhere near 1.7 to 2.0 MeV by theoretical means, so the calculation actually yields numbers 4 to 5 MeV short of experiment.

The uncertainty can be partially removed by considering the binding energy of the last two nucleons, which occupy the $0p$ orbits, relative to the α-particle core. In this case the Coulomb effect may be deducted from the experimental values by standard shell model procedures.[9,16,17] The results appear in the third and fourth data columns of Table I. Correspondence between theory and experiment is now considerably better, with most discrepancies ranging from 0.3 to 0.5 MeV. An exception is the second $J=1$, $T=0$ level which appears at an excitation energy of 6.00 MeV. This state needs special attention, and will be discussed later in this section. The improved comparison between theory and experiment is seen for two reasons. First, the binding energy of the last two nucleons is simply less sensitive since it involves the interaction of a smaller number of pairs of particles. More important, the greatest source of error in the calculation lies in the α-particle core. The α-particle binding energy was found[11] to be nearly 4 MeV short of experiment, and this discrepancy comes through in all calculations in the present work.

The final pair of columns in Table I compares the computed energy level spectrum with experiment. In this case agreement is very good, discrepancies are only on the order of 0.2 MeV except in the second $J=1$, $T=0$ level.

The problem with the $J=1$, $T=0$ state at 6.00 MeV is that it has absolute quantum numbers identical to the ground state. In a variational calculation a rigorous upper bound is obtained only when one calculates the ground state, or when the calculated state is guaranteed to be orthogonal to all levels lying lower in energy within the system. There is no problem with the first four excited states in ^{6}Li, since all have different sets of absolute quantum numbers (J,T) and orthogonality is ensured. In order to obtain an upper bound on the 6.00 MeV level one would have to ensure orthogonality to the *true* ground state wave function. In the present example this is clearly impractical since this true wave function is unknown. An alternative is to simply require the excited state wave function to be orthogonal to the approximate ground state function obtained in the calculation, but this has never been shown to be generally satisfactory.[19]

In the present investigation the second $J=1$, $T=0$ state was simply calculated in two different ways, in order to estimate the uncertainty in the eigenvalue. First, the shell model matrix elements obtained in the ground state calculation were used to compute the second root of the shell model Hamiltonian in the model space. This ensures that the model space portions of the wave functions for the first and second $J,T=1,0$ levels are orthogonal. Table I shows that this produces an energy which is 0.72 MeV too high in the excitation spectrum. Second, the calculation for the 6 MeV level was redone self-consistently, that is by iterating U and the C_i. This is clearly the better procedure of the two, and yielded an energy eigenvalue improved by 0.21 MeV. Neither eigenvalue represents a rigorous upper bound, and consequently both are suspect.

The effective shell model matrix elements

$$\langle 0p^2LSJT \mid v_{12}^{\mathrm{SM}} \mid 0p^2L'S'JT\rangle \tag{38}$$

TABLE I. Calculated results for the low lying energy levels of ^{6}Li, compared with experiment. All energies are in MeV.

	Total binding energies[a]		Energy eigenvalues relative to the ^{4}He core[b]		Excitation energies	
JT	Exp	Calc	Exp	Calc	Exp	Calc
10	31.99	29.70	−4.69	−4.20	0	0
30	29.81	27.74	−2.51	−2.24	2.18	1.96
01	28.43	26.27	−1.13	−0.77	3.56	3.43
20	27.42	25.30	−0.12	0.20	4.57	4.40
21	26.63	24.47	0.67	1.03	5.36	5.23
10[c]	25.79	22.98	1.31	2.52	6.00	6.72
(10)[d]		(23.19)		(2.31)		(6.51)

[a]Coulomb energy was neglected in the calculation, but cannot be (unambiguously) deducted from the experimental values. This will enhance disagreement by about 1.7–2.0 MeV.

[b]Coulomb energy was not included in the calculation, and was deducted from the experimental results by standard shell model methods.

[c]The second $J,T=1,0$ level was calculated without self-consistent reevaluation of the variational parameters.

[d]The second $J,T=1,0$ level recalculated self-consistently.

TABLE II. Comparison of the matrix elements $\langle 0p^2LSJT \mid V_{12}^{SM} \mid 0p^2L'S'JT \rangle$ deduced in the present work with previous calculations, in MeV.

JT	LS	$L'S'$	Cohen-Kurath	Norton-Goldhammer	Tripathi-Goldhammer	Sussex Group	Paris potential
21	^1D	^1D	−3.05	−3.40	−3.67	−2.42	−2.58
	^1D	^3P	−0.50			−0.35	0.46
	^3P	^3P	1.27	0.04	−0.39	0.32	−1.98
11	^3P	^3P	0.86	2.36	−0.64	−0.29	1.67
01	^3P	^3P	4.33	0.22	2.08	1.32	6.93
	^3P	^1S	−0.33			−0.08	−0.21
	^1S	^1S	−6.73	−5.65	−5.38	−5.09	−5.36
30	^3D	^3D	−6.88	−5.57	−5.32	−5.14	−5.02
20	^3D	^3D	−4.23	−6.02	−6.81	−6.06	−6.28
10[a]	^3D	^3D	−5.20	−7.79	−4.22	−5.05	−5.97
	^3D	^3S	−1.33	−1.09	−1.05	−0.82	−1.19
	^3D	^1P	−0.73			−0.19	−0.35
	^3S	^3S	−8.81	−9.82	−8.62	−8.66	−8.94
	^3S	^1P	−0.30			−0.34	−0.44
	^1P	^1P	0.07	7.13	1.92	0.26	2.86

[a]These $J=1$, $T=0$ matrix elements were deduced from the ground state calculation.

deduced in this calculation are shown in Table II. Comparison is made there with the corresponding matrix elements obtained in the shell model χ^2 fits of Cohen and Kurath[16] and Norton and Goldhammer,[17] the G-matrix calculation of Tripathi and Goldhammer,[18] and the perturbation calculation of the Sussex[9] group. Of these, the Sussex calculation lies the closest in general philosophy to the present work. Considerable agreement among the various methods is seen for many of the matrix elements, but the areas of disagreement are more interesting. The most prominent of these are in the matrix elements involving the ^3P states.

The reason appears to lie in the very strong spin-orbit interaction present for odd parity states in the Paris potential. This is an important effect, and some effort was made to cross check the result. First, the Reid[21] potential was examined. There, as in the Paris potential, one finds a very strong spin orbit interaction in the odd parity states as opposed to a relatively weak one in even parity states. This appears to be characteristic of realistic nuclear forces. Why did it not appear in the G-matrix calculation of Tripathi and Goldhammer with the Hamada-Johnston potential?[18] The problem may lie in the fact that the two-body spin-orbit interaction is of very short range, and hence quite sensitive to the behavior of the wave function as two particles come very near to each other. The hard core potentials may force the wave function to zero too fast, thus underestimating the spin orbit interaction.

Table III shows the single particle energies for the $p_{3/2}$ and $p_{1/2}$ orbitals deduced from the calculation of ^{5}He. The doublet splitting obtained with the Paris potential is seen to be in good agreement with experiment. The reason for this fairly large splitting is primarily due to the strong spin orbit interaction discussed above. The tensor force in the Paris potential is relatively weak, and consequently accounts for only about 1.3 MeV of this doublet splitting.

Table IV contrasts shell model matrix elements for a self-consistent calculation of the ground state, with the corresponding elements for the excited $J=1$, $T=0$ level. The changes in these matrix elements are seen to be quite small. The largest alteration is the $^3S_1$ state, and is only 0.33 MeV; while the $^1P_1$ diagonal matrix element does not change at all within the accuracy of the calculation. The

TABLE III. Single particle energies in MeV (obtained for ^{5}He) for the $p_{3/2}$ and $p_{1/2}$ orbitals.

Method	$\epsilon(p_{3/2})$	$\epsilon(p_{1/2})$
Cohen-Kurath	1.63	2.27
Norton-Goldhammer	1.31	5.21
Tripathi-Goldhammer	5.4	7.0
Sussex	3.63	5.66
Present work	1.39	5.29
Experiment	0.95	5.0±1.5[a]

[a]The experimental position of the $p_{1/2}$ level in ^{5}He is not very well determined, and even the error quoted above is an approximation gleaned from several experimental papers (Ref. 20).

TABLE IV. Comparison of matrix elements with $J=1$, $T=0$ by self-consistent calculations on the ground state, and then on the 6.00 MeV excited state. The latter values are in parentheses. All energies are in MeV.

	^3S	^3D	^1P
^3S	−8.94	−1.19	−0.44
	(−8.61)	(−1.14)	(−0.39)
^3D		−5.97	−9.35
		(−6.19)	(−0.31)
^1P			2.86
			(2.86)

difference reflects the fact that configuration mixing is far more important in the S states.

It must be remembered that the shell model matrix elements are by no means unique. Like any set of potential matrix elements one can, of course, always make a unitary transformation to obtain a different set. In the case of an effective interaction in a truncated model space one has considerably more latitude. The interaction parameters will depend on precisely how the model basis is defined. As a simple example one could change the oscillator size parameter in the calculation, thereby obtaining a new set of basis functions with an altered shell model interaction.[9] More complex alterations are clearly possible. For example, one could take the $1s\,0d$ orbitals out of the excited states in this calculation, and insert them into the model space. Under such an operation the matrix elements for the $0p$ orbitals would certainly be altered. It is interesting that the various shell model interactions shown in Table II show so much agreement in many of the matrix elements in spite of these complications.

IV. CONCLUSION

The main source of error in this work appears to lie within the calculation of the α-particle core. This may be considered additional evidence that the discrepancies in the α-particle calculation are due to the absence of three-body correlations in the wave function and three-body nuclear forces in the calculation. These effects will be smaller in the ^{6}Li spectra, and one may have some cancellation when energy differences are computed.

The most encouraging feature of the results is that the generalization of the trial wave function to a degenerate model space evidently produced no new errors. There is the problem of calculating a second excited level with the same absolute quantum numbers of a lower state, but this is an old difficulty which we did not expect to resolve in this paper.

A sample of the variational parameters (K_i) found for the ^{6}Li ground state are shown in Table V. The $^3S_1$ and $^1S_0$ partial waves shown belong to the central perturbed $0s$ oscillator state, while the $^1P_1$ channel parameters perturbed the $0p$ state. The values previously[11] obtained for the α particle with the Paris potential are also shown, merely to show that there is very little change in these parameters due to the channel coupling introduced by two additional nucleons in the $0p$ shell. The interesting feature to be noted in this table is the rapid fall off in magnitude of the K_i with increasing β for the ^1P state as compared with the S states.

TABLE V. A sample of the variational parameters (K_i) obtained for the ground state of ^{6}Li. In the $^1S_0$ and $^3S_1$ channels the corresponding parameters previously (Ref. 11) obtained in the α-particle calculation are shown for comparison.

β	$K(^3S_1)$		$K(^1S_0)$		$K(^1P_1)$
0.1	−1.762	(−1.539)	−1.958	(−1.852)	0.742
0.3	0.934	(1.009)	1.972	(1.980)	0.213
0.5	1.026	(1.182)	0.519	(0.517)	0.078
0.7	1.491	(1.538)	2.493	(2.500)	0.042
0.9	5.009	(5.017)	2.949	(2.953)	0.008

Smaller values of β correspond to low energy excitations. The relatively large values of K_i for $\beta=0.9$ in the S states indicates that one is including a considerable admixture of very highly excited oscillator orbitals in the perturbed wave function for those states. This well-known effect is required in order to force the perturbed wave function toward zero at small nucleon-nucleon separations in order to accommodate the strong short range (high momentum) repulsion in modern interaction operators.

In the p states, and in states of higher angular momentum, the wave function near the origin is zero from the start. Consequently, the high energy excitations compose a much smaller admixture into the perturbed wave function, and most of the excitations appear to be of $2\hbar\omega$ and $4\hbar\omega$. No attempt was made to exploit this simplicity in the present calculations.

There are some obvious ways to improve upon the variational wave function employed here. One could extend the model space to include the states excited by $2\hbar\omega$ over the $(0s)^4\,(0p)^2$ configuration used in this paper. This will lead to a very large zero-order basis, however, and seems to be quite unwieldy. An alternative would be to introduce three-body operators (W_{ijk}) into the trial wave function of Eq. (11). This procedure seems much more tractable within the procedures developed so far for this method, but will certainly require considerably more effort and computer time. It is not likely that definitive results could be obtained in this manner until three-body nuclear forces are reasonably well known.

Lastly, there could be room for improvement through refinement of the two-body operators used in Eq. (11).

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