Abstract

We adopt a personal approach here reviewing several calculations over the years in which we have experienced confrontations between cluster models and the shell model. In previous cluster conferences we have noted that cluster models go hand in hand with Skyrme Hartee-Fock calculations in describing states which cannot easily, if at all, be handled by the shell model. These are the highly deformed (many particle - many hole) intruder states, linear chain states e.t.c. In the present work we will consider several topics; the quadrupole moment of $^6$Li, the non-existence of low lying intruders in $^8$Be, and then jumping to the $f_{7/2}$ shell, we discuss the two-faceted nature of the nuclei - sometimes displaying shell model properties, other times cluster properties.

I. THE QUADRUPOLE MOMENT OF THE J = 1$^+$ STATE IN $^6$LI

Whereas the quadrupole moment of the deuteron is positive ($Q = +2.74$mb), that of the J=1$^+$ state of $^6$Li is negative, $Q=-0.818(17)$mb. The magnetic moment of the deuteron is $\mu = 0.85741$ nm while that of $^6$Li is 0.822 nm.

There appears to be a big discrepancy between cluster model calculations and the shell model calculations. In nearly all cluster model calculations $Q$ comes out positive. However in many shell model calculations $Q$ comes out negative, sometimes too negative. This is an important problem that deserves further attention. See for example arguments in the literature between the cluster group[1] and the shell model group[2]. See also the recent compendium of A=6 by D.R. Tilley et. al.[3].
For example in a modern shell model approach by Forest et. al. [4] gets about -8 mb for Q, a factor of 10 too large but of the correct sign. On the other hand in a dynamical microscopic three cluster description of $^6$Li where the clusters are $\alpha$, n, and p the result is $Q = 2.56$ mb.[1]

In shell model calculations that we performed [5] we started with 2 valence particles in the 0p shell ($0\hbar\omega$). Then we allowed up to 2 $h\omega$ and then up to 4 $h\omega$ excitations. In the $0\hbar\omega$ space if you do not have a tensor interaction Q comes out positive. With a 'realistic' tensor interaction Q comes out negative but too negative $Q=-3.5$mb. However with a former student Zheng, who at Arizona also developed the no core approximation with Barrett et. al.[6], we showed that when higher shell admixtures were admitted Q became smaller in magnitude and closer to experiment as shown in the following table.[5]

The results are shown in the following table

| SPACE | Q(mb) | $\mu$(mm) |
|-------|-------|-----------|
| $0\hbar\omega$ | -3.60 | 0.866 |
| $2\hbar\omega$ | -2.51 | 0.848 |
| $4\hbar\omega$ | -0.085 | 0.846 |
| Experiment | -0.82 | 0.822 |

Note that the shell model calculations cannot get the magnetic moment low enough. With up to 4 $h\omega$ admixtures we actually overshoot and get a quadrupole moment that is too small but still negative. Some cluster models appear to explain the low magnetic moment.

An excellent discussion of many shell model calculation of Q and $\mu$ has been given by Karatatlidis et. al [7]. The value of Q that they obtain with what they call the “Zheng” interaction [8] in the up to 0,2,4 and 6 $h\omega$ spaces are -2.64,-2.08,-0.12, and 0.17 mb respectively. Thus they get Q to become positive at the 6 $h\omega$ level. But then they quote Zheng et. al [8] as getting a value of -0.67mb in the same 6 $h\omega$ space. It is not clear why the two calculations give different answers. The changes in $\mu$ in ref [7] are more moderate 0.869,0.848, 0.845 and 0.840 mm in the up to 0,2,4 and 6 $h\omega$ spaces.

Looking at all the calculations by all groups (including our own), the situation is certainly confusing, and the problem deserves further attention. This is certainly a basic problem, the deuteron embedded in the nuclear medium. This problem has wider implications whether or not there is T=0 pairing can depend on how higher order configurations affect the tensor interaction in the valence space.
II. ABSENCE OF LOW LYING INTRUDERS IN $^8$Be AND THE $\alpha$ PARTICLE MODEL

The $0^+$ bandhead for low lying intruders in $^{16}$O, $^{12}$C, and $^{10}$Be are at 6.05 MeV, 7.65 MeV and 6.18 MeV respectively. In $^{16}$O and $^{12}$C, these are predominantly 4 particle 4 hole excitations. In $^{12}$C, we identify the intrinsic state as a linear chain. In the 7th edition of the 'Tables of Isotopes' possible intruders in $^8$Be were indicated, a J=$0^+$ state at 6 MeV and J=$2^+$ state at 9 MeV.

In shell model calculations allowing 2 particle 2 hole excitations we were able with a quadrupole-quadrupole force to get a J=$0^+$ state at 9.7 MeV in $^{10}$Be, too high but in the right ballpark.[7,8] But we could not get low lying intruders in $^8$Be below 30 Mev.[7,8] We used a deformed oscillator model to show why one gets intruders in $^{12}$C and $^{10}$Be but not $^8$Be.

But perhaps the simplest explanation as suggested to us by E. Vogt is given by the $\alpha$ particle model. In $^{12}$C we can rearrange the $\alpha$ particles from a triangle to a linear chain. In $^8$Be we have only 2 $\alpha$ particles. One can get a rotational band by having the 2 $\alpha$’s rotate around each other but that is all.

The mere existence of these intruder states is of astrophysical importance. In the beta decay $^8$B+$\rightarrow$ $^8$Be + $e^+$ + $\nu$ one goes from a J=$1^+$ T=1 to J=$2^+$ states. This is the famous 'Ray Davis' neutrino. If there were a $2^+$ state at 9 MeV then there would be more high energy $\alpha$’s than there would be if the decay were to the $2^+$ at 3.04 MeV.[9] The alpha spectrum from the decay of $^8$Be seems to show more high energy alphas, but we would say that they are not due to low lying intruders.

III. CLUSTERING AND SHELL MODEL IN THE $F_{7/2}$ REGION

In a previous cluster conference in Santorini (1993) a spectrum of $^{44}$Ti was shown in an $\alpha$ cluster model.[10] The spectrum looked reasonable except that there was a wide gap between the $10^+$ and $12^+$ states. However, these states are sufficiently close together that the $12^+$ state is isomeric. In a single j shell basis (j=$f_{7/2}$) $^{52}$Fe is the 4 hole system and it should have an identical spectrum to that of $^{44}$Ti provided the same interaction is used. However in $^{52}$Fe the $12^+$ lies below the $10^+$ state. It is extremely isomeric and has a lifetime of 12 minutes.

We have studied this and other topics by calculating the spectrum of $^{44}$Ti ($^{52}$Fe) with a variety of interactions designated as Model X. (See Tables I,II)
Model I: Use the spectrum of $^{42}$Sc as input (particle-particle) Identify $< (j^2)^l V(j^2)^l > = E(J)$ experimental. For isospin T=0 J can be 1,3,5 and 7 while for T=1 J is even 0,2,4, and 6.

Model II: Use the spectrum of $^{54}$Co as input (hole - hole). If there were no configuration mixing these two spectra would be identical. However, there are some differences eg the $7^+$ state is much lower in $^{54}$Co than in $^{42}$Sc.

Model III: Now we play games. We want to find out how important are the T=0 matrix elements for the structure of the nuclei. (e.g. Is T=0 pairing important?) Noticing that in $^{42}$Sc the J=2,3 and 5 states are nearly degenerate in this model we set all the T=0 matrix elements to be the same and to all equal $E(2^+) = 1.5863$ MeV.

In model III we then have $V^{T=1} = V(^{42}Sc)^{T=1} J =0,2,4,6$ and $V^{T=0} =$ constant$= E(2^+)$ $J=1,3,5,7$. We can then write $V^{T=0} =$ constant $= (1/4 - t_1 \cdot t_2)$. We can then write $V^{T=0} = c(1/4-t_1 \cdot t_2)$ where c is a constant. Hence $\sum_{i<j} V^{T=0}_{ij} = c/8(n(n-1)+6) - c/2T(T+1)$. This means that the spectrum of states of a given isospin e.g. T=0 in $^{44}$Ti($^{52}$Fe) is independent of what the constant is, it might as well be zero. Of course the relative splitting of T=1 and T=0 states will be affected. Model III will be the standard from which we derive Model IV.

Model IV: Relative to the degenerate case above, we now move the $J = 1^+$ state down in energy to 0.5863 MeV. Our motivation is based on numerous discussions about the importance of T=0 S=1 “pairing” in nuclei. We hope to simulate the T=0 pairing by this lowering.

Model V: Relative to Model III we bring the J=1$^+$ and J=7$^+$ states down to an energy of 0.5863 MeV but keep the J=3$^+$ and 5$^+$ at $E=E(2^+)=1.5863$ MeV. This spectrum is very close to that of $^{42}$Sc.

IV. DISCUSSION OF RESULTS

Let us first compare Model III (all T=0 matrix elements are degenerate) with Model I (spectra of $^{42}$Sc). As already mentioned, making T=0 matrix elements degenerate is equivalent to making them zero as far as T=0 states are concerned.

The main difference is that the states with J=6,4,7, and 8 come down in energy as does J=9$^+$. Also the 12-10 gap is a bit greater than for the $^{42}$Sc spectra case, reminiscent of the $\alpha$ particle model. The J=9$^+$ state is below the 10$^+$ and 12$^+$ in the degenerate case. Clearly it is the high energy side of the spectrum which is most sensitive to the change from experimental spectrum to the “T=0 degenerate” case.
Despite the changes, we can say that the T=1 two body matrix elements give the dominant structure of the spectrum whilst the T=0 matrix elements provide the fine tuning.

We now compare Model IV with Model III. The only difference is that we break the T=0 degeneracy by lowering the J=1+ state from 1.5863 MeV to 0.5863 MeV. We hope that this simulates to some extent T=0 S=1 neutron-proton pairing. The change from degenerate case is not that large. There is a tendency to go towards the spectrum of 42 Sc. The J=3,5,7, and 8 states are raised somewhat in energy. However it is hard to find a clear signature of this S=1 pairing.

Not shown is Model V where we bring down both the J=1+ and 7+ states to 0.5863 MeV keeping J=3 and 5 at E(2) = 1.5863 MeV. This input spectrum is close to that of 42 Sc so that it is not surprising that the 44 Ti spectrum is likewise close.

We lastly consider the results using the spectrum of 54 Co. This was done some time ago by Geesaman [11,12] Note that there are significant changes, all at the high energy high angular momentum part of the spectrum. Relative to the 42 Sc case the 10+ and 12+ states are down in energy with the 12+ below the 10+ thus leading to a long lifetime for the 12+ state. Note that the 9+ state is now at a much high energy than the 10+ or 12+. Recently the 10+ state in 52 Fe, which lies above the 12+ has been found in 52 Fe by Ur et. al. [13]. It would also be of interest to find the 9+ state.

V. MANY PARTICLE, MANY HOLE STATES IN 40 CA

This is a topic we discussed in previous cluster meetings so we will be brief.[14] We just want to remind the reader that there are all sorts of many particle-many hole highly deformed states in 40 Ca. One cannot properly describe 40 Ca in a cluster model consisting of 36 Ar plus an alpha particle. At the very least one has to start with 32 S plus two alpha particles.

In a Skyrme Hartree-Fock calculations (SK III) we obtain a near degeneracy of the 4p-4h and 8p-8h intrinsic state. The respective energies are 12.1 MeV and 11.4 MeV. The 8p-8h intrinsic state energy is lower than the 4p-4h. By the time projection and pairing are included, the 4p-4h comes lower than the 8p-8h (6.85 MeV vs 8.02 MeV) in agreement with the order the J = 0 excitation energies of 3.0 and 5.1 MeV. Pairing will lower the states even more. We actually found many more deformed states of the form np-nh n=2,3,4,5,6,7 and 8. The intrinsic states are nearly degenerate in energy - we called this a deformation condensate. We also found for these states that the deformation parameter was approximately proportional to n i.e. the value of β for 8p-8h is approximately twice the value of β
for 4p-4h.

In $^{80}$Zr one of the np-nh states becomes the ground state. This is the 12p-12h state which has a calculated value of $\beta = 0.4$ A more superdeformed 16p-16h state with $\beta = 0.6$ is calculated to be at an excitation energy of about 8 MeV.

VI. TWO DIFFERENT VIEWS OF THE $F_{7/2}$ REGION

In March 2000 issue of the Physical Review C 61 there are two papers side by side. One is by our group [15] and one by H. Hasegawa and K. Koneko [16]. We both do calculations in the $f_{7/2}$ shell. We emphasize shell model behavior whilst the other authors the $\alpha$ cluster behaviors, even though their model space is limited to $f_{7/2}$.

The other authors point out that we can get an excellent approximation to the ground states of $n_p = n_n = 2m$ nuclei ($n_p$ is the number of protons e.t.c.).

$$|(f_{7/2})^{4m}I = T = 0 >= \frac{1}{\sqrt{N_0}}(\alpha_0^\dagger)^m |A_0 >$$

where $(\alpha_0^\dagger)$ creates a 4 nucleon cluster.

$$\alpha_0^\dagger = \sum_{J,\tau} (J, J : I = T = 0)(A_{J, \tau}^\dagger A_{J, \tau}^\dagger)_{I=0T=0}$$

For $^{48}$Cr this approximation give -32.04 MeV for the ground state energy whereas the exact value is 32.70 MeV.

We on the other hand have emphasized the shell model aspects.[15] In the previously mentioned paper, we find an approximation for the excitation energies of single and double analog states in the $f_{7/2}$ region and in an earlier paper “Fermionic Symmetries: Extension of the two to one relationship between spectra of even even and neighboring odd mass nuclei”[17] we noted two things.

A. There is often a two to one relation between spectra of even-even and even odd nuclei, and in some cases the single j shell model predicts this.

B. Excitation energies of analog state are approximately the same if the neutron excess (or equivalently the ground state isospin) is the same.

The above results can be parametrized by the following formulae

SINGLE ANALOG EXCITATION (SA)

$$E(SA) = b(T + X)$$

DOUBLE ANALOG EXCITATION (DA)
$E(DA) = 2b(T + X + 1/2)$ \hspace{1cm} (4)

This formula will give a two to one ratio for $E(DA)/E(SA)$ for $(^{44}\text{Ti},^{43}\text{Ti})$, $(^{51}\text{Cr},^{50}\text{Cr})$, $(^{47}\text{Sc},^{48}\text{Ti})$ etc.

The experimental SA and DA are shown in the following table.

\begin{align*}
T=0 & \quad ^{44}\text{Ti} (9.340), \quad ^{48}\text{Cr} (8.75), \quad ^{52}\text{Fe} (8.559) \\
T=1/2 & \quad ^{43}\text{Sc} (4.274)^a, \quad ^{43}\text{Ti} (4.338)^a, \quad ^{45}\text{Ti} (4.176), \quad ^{49}\text{Cr} (4.49), \quad ^{51}\text{Mn} (4.451), \quad ^{53}\text{Co} (4.390), \quad ^{53}\text{Fe} (4.250) \\
T=1 & \quad ^{46}\text{Ti} (14.153), \quad ^{50}\text{Cr} (13.222) \\
T=3/2 & \quad ^{45}\text{Sc} (6.752)^a, \quad ^{47}\text{Ti} (7.187), \quad ^{51}\text{Cr} (6.611) \\
T=2 & \quad ^{48}\text{Ti} (17.379) \\
T=5/2 & \quad ^{47}\text{Sc} (8.487)^a, \quad ^{49}\text{Ti} (8.724) \\
^a & \quad \text{obtained from binding energy data.}
\end{align*}

In Table II we compare the theoretical single j shell calculations with the linear formula. We take $b = 2.32$ MeV $X=1.30$. Note that in the SU(4) limit $X=2.5$. The fact that SU(3) gives the linear formula is not sufficient for it to be the correct theory. For a simple monopole-monopole interaction $a+bt(1)t(2) X=1$.

Some of the two to one ratio’s hold rigously in the single j shell model. This holds for 3 particle and 4 particle systems or 3 holes and 4 holes. eg $(^{43}\text{Ti},^{44}\text{Ti}), (^{43}\text{Sc},^{44}\text{Ti}), (^{53}\text{Fe},^{52}\text{Fe})$. Here not only single or double analog but all the J=j states in the odd spectrum are at half the energy of the J=0+ states in the even system.

Some of the relations hold approximately in the single j shell model eg for $(^{45}\text{Sc},^{46}\text{Ti})$ and for the cross conjugate pair $(^{51}\text{Cr},^{50}\text{Cr})$ we would get a 2 to 1 ratio if seniority four states could be neglected and one only had $v=0$ and $v=2$.

Miraculously the 2 to 1 ratio holds remarkably well experimentally for $(^{51}\text{Cr},^{50}\text{Cr})$ - the values are 6.511 and 13.022 MeV respectively, this despite the fact that in the single j shell it should only hold approximately.Ironically the simplest system for which 2 to 1 should hold exactly does not work so well. That is to say for $(^{43}\text{Ti},^{44}\text{Ti})$ the values are 4.338 and 9.340 MeV. When configuration mixing is included, agreement with the deviation is explained. This might be an example of a 4 particle clustering. For the hole system $(^{53}\text{Fe},^{52}\text{Fe})$ on the other hand 2 to 1 works much better.

The fact that there is in general a close relation between even-even and even-odd puts to question whether in those many cases there is any $\alpha$ particle clustering.

The single j shell calculation does not predict exact equality for the S.A. excitation energies in $^{43}\text{Sc}$ and $^{45}\text{Ti}$. The relative values are very close however 4.142 and 4.112 MeV respectively. This is fascinating. We take $^{43}\text{Sc}$, jam a deuteron into it to form $^{45}\text{Ti}$ and it
seems hardly to make any difference for S.A. excitations.[15]

VII. TWO VIEWS OF CROSS CONJUGATE RELATIONS

In the single j shell model, the spectra of cross conjugate nuclei should be identical.[18] (for j^n states.). A cross conjugate nucleus is one obtained by changing protons into neutron holes and neutrons into proton holes. The cross conjugate of 46Ti is 50Cr. Let us compare the spectra

| J   | 46Ti | 50Cr | Ratio   |
|-----|------|------|---------|
| 0   | 0.000| 0.000|         |
| 2   | 0.889| 0.787| 0.8853  |
| 4   | 2.010| 1.884| 0.9373  |
| 6   | 3.297| 3.164| 0.9597  |
| 8   | 4.896| 4.740| 0.9681  |

The fits are very good. The 50Cr excitations are slightly smaller - it could be a universal A dependence. Where does the remarkable agreement leave room for α clustering?

However we can look for other things besides the spectra. In a recent experiment theory collaboration where the leading experimentalists were N. Koller and H.A. Speidel [19] good agreement was obtained for g(2^+) in 50Cr but bad agreement for 46Ti. The shell model predicts a high value of g(2^+) and g(4^+) for 50Cr but low values for 46Ti 0.25 mm. The high values are confirmed for 50Cr but for 46Ti the measured g factors are closer to 0.5 which suggest the rotational value g_R=Z/A. These results suggest that there must be considerable clustering in 46Ti that is not present in 50Cr. In general the shell model appears to work better in the upper half of the “f_{7/2} shell” than in the lower half. There appears to be much more going on in the lower half and probably this is due to intruder/cluster mixing in with the basic shell model states.

VIII. CLOSING REMARKS

We have provided several examples where Cluster Models and the Shell Model confront each other usually to the mutual benefit of both models even though in the short term there might be some arguments. The two models give the opposite sign for the quadrupole moment of 6Li, and this has to be resolved. The cluster model provides insight into some results of detailed shell model calculations e.g. why there are no low lying intruders in 8Be. The low lying intruder states e.g. 4p-4h and 8p-8h in 40Ca are essentially impossible
to calculate in the shell model. However here cluster models and Skyrme-Hartree Fock go
together in describing such states. In the f_{7/2} region we raise the question (without fully
answering it) of how to distinguish symmetry energy from clustering energy. Finally we
point out the issue of hidden clustering.

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Ti 44 spectra for Models I,II,III, and IV

Model I  Model II  Model III  Model IV
TABLE I. Two particle Matrix Elements \( <(j^2)^{J'} V(j^2)^{J'} > \)

| Case   | J=0 T=1 | J=2 T=1 | J=4 T=1 | J=6 T=1 | J=1 T=0 | J=3 T=0 | J=5 T=0 | J=7 T=0 |
|--------|---------|---------|---------|---------|---------|---------|---------|---------|
| Model I\(^{(a)}\) | 0.000   | 1.5863  | 2.8153  | 3.2420  | 0.6110  | 1.4904  | 1.5101  | 0.6163  |
| Model II\(^{(b)}\)  | 0.000   | 1.4465  | 2.6450  | 2.9000  | 0.9372  | 1.8224  | 2.1490  | 0.1990  |
| Model III\(^{(c)}\) | 0.000   | 1.5863  | 2.8153  | 3.2420  | 1.5863  | 1.5863  | 1.5863  | 1.5863  |
| Model IV\(^{(d)}\) | 0.000   | 1.5863  | 2.8153  | 3.2420  | 0.5863  | 1.5863  | 1.5863  | 1.5863  |

TABLE II. \(^{44}\)Ti \(^{(52}\)Fe) spectra for Model I,II,III and IV

| Model I \((J^\pi E)^{(a)}\) | Model II \((J^\pi E)^{(b)}\) | Model III \((J^\pi E)^{(c)}\) | Model IV \((J^\pi E)^{(d)}\) |
|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| 0\(^+\) 0.000               | 0\(^+\) 0.000               | 0\(^+\) 0.000               | 0\(^+\) 0.000               |
| 2\(^+\) 1.163               | 2\(^+\) 1.015               | 2\(^+\) 1.303               | 2\(^+\) 1.253               |
| 4\(^+\) 2.790               | 4\(^+\) 2.628               | 4\(^+\) 2.741               | 4\(^+\) 2.800               |
| 6\(^+\) 4.062               | 6\(^+\) 4.079               | 6\(^+\) 3.500               | 6\(^+\) 3.738               |
| 3\(^+\) 5.786               | 8\(^+\) 5.772               | 3\(^+\) 4.716               | 3\(^+\) 5.031               |
| 5\(^+\) 5.871               | 7\(^+\) 6.018               | 5\(^+\) 4.998               | 5\(^+\) 5.082               |
| 7\(^+\) 6.043               | 12\(^+\) 6.514              | 7\(^+\) 5.356               | 7\(^+\) 5.687               |
| 8\(^+\) 6.084               | 3\(^+\) 6.540               | 8\(^+\) 5.656               | 8\(^+\) 6.045               |
| 10\(^+\) 7.384              | 5\(^+\) 6.602               | 9\(^+\) 7.200               | 9\(^+\) 7.731               |
| 12\(^+\) 7.702              | 10\(^+\) 6.722              | 10\(^+\) 7.200              | 10\(^+\) 7.731              |
| 9\(^+\) 7.984               | 9\(^+\) 8.048               | 12\(^+\) 7.840              | 12\(^+\) 8.371              |

\(^{(a)}\) Input is spectrum of \(^{42}\)Sc(particle-particle)
\(^{(b)}\) Input is spectrum of \(^{54}\)Co(hole-hole)
\(^{(c)}\) The T=1 matrix elements are from the spectrum of \(^{42}\)Sc. The T=0 matrix elements are degenerate at 1.5863 MeV.
\(^{(d)}\) Same as model 3 except that the J=1\(^+\)T=0 energy is lowered to 0.5863 MeV.
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