Linear approximation for the excitation energies of single and double analog states in the $f_{7/2}$ shell

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We find that the excitation energies of single analog states for odd-even nuclei in the $f_{7/2}$ shell with $J=j=7/2^-$ and the $J=0^+$ double analog states in the even-even nuclei are fairly well described by the formulas $E^*(j,T+1)=b(T+X)$ and $E^*(0^+,T+2)=2b(T+X+0.5)$, respectively, where $T=|N-Z|/2$ is usually the ground-state isospin. Comparisions are made with single *j*-shell calculations and also those involving configuration mixing.

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In a 1964 Technical Report, McCullen, Bayman, and Zamick (MBZ) gave the wave functions and energy levels for nuclei in the $f_{7/2}$ shell [1]. They noted in their single *j*-shell calculations, that in some cases there was a two to one relation between the spectra of even-even nuclei and neighboring odd A nuclei. For example, the calculated $J=0^+$ spectra of ^{44}Ti, were at twice the energies of the corresponding $J=j$ levels in ^{43}Ti (or ^{43}Sc). The same was true for the pairs (^{48}Ti,^{47}Sc), (^{48}Ti,^{49}Ti), and (^{52}Fe,^{53}Fe). That the two to one relation should hold can easily be proved [2]. For these nuclei the two to one relation holds for all levels (of the j^n configuration) which also includes the double and single analog states. It was noted by Zamick and Zheng [3] that the two to one relation holds quite well experimentally not only for the above-mentioned pairs but for others as well. Zamick and Devi showed [2] that this relation also holds *approximately* for (^{46}Ti,^{45}Sc) and the cross conjugate pair (^{50}Cr,^{51}Cr). One gets an exact two to one relation here as well if one excludes seniority four states.

Besides the two to one relation there are some general systematics of the excitation energies of the single analog (SA) states and double analog (DA) states, observed for nuclei in the f-p shell. In Table I, we give the relevant data where the nulcei with the same absolute value of the neutron excess $|N-Z|$, or what is equivalent to the ground-state isospin $T=|N-Z|/2$, are grouped together. The theoretical analysis of these systematics will be given in the next section. For some nuclei (^{43}Sc,^{45}Sc,^{47}Sc,^{43}Ti) the excitation energies of SA states have not been measured. In such cases we can get a very good estimate of these energies from the nuclear binding energies. For example,

$$E(\mathrm{Sc}^{43})_{T=3/2}-E(\mathrm{Sc}^{43})_{T=1/2} = E(\mathrm{Ca}^{43})+E(\mathrm{Sc}^{41})-E(\mathrm{Ca}^{41})-E(\mathrm{Sc}^{43})_{T=1/2},$$

where E is minus the binding energy.

The experimental data given in Table I, and some soon to be discussed calculations suggest an approximate linear fit to the excitation energies of SA and DA states

$$E(\mathrm{SA})=b(T+X).$$

In order to get a two-to-one ratio for the selected DA to SA analog excitation energies, one would have

$$E(\mathrm{DA})=2b(T+X+1/2).$$

For a simple monopole interaction $a+bt(1)\cdot t(2)$ the SA energy will be

$$\frac{b}{2}[(T+1)(T+2)-T(T+1)]=b(T+1),$$

and the DA energy would be

$$\frac{b}{2}[(T+2)(T+3)-T(T+1)]=2b(T+3/2).$$

Thus for this simple interaction $X=1$. In general, X need not be equal to one. For example, in the SU(4) limit one can show that the isospin-dependant term in the binding energy formula is proportional to $T(T+4)$. This corresponds to $X=2.5$.

We now present the single *j*-shell results. These are the same as the MBZ results except that we now have a better knowledge of the $T=0$ matrix elements $\langle(j^2)^I|V|(j^2)^I\rangle$ which are obtained from the spectrum of ^{42}Sc. The results are shown in Table II. The input matrix elements in MeV are 0, 0.6111, 1.5863, 1.4904, 2.8153, 3.242, and 0.6163 respectively, for $I=0,1,\ldots,7$.

We find that we get a good fit to the single *j*-shell results with $b=2.32$ MeV and $X=1.30$. This value of X differs significantly from the value in the SU(4) limit. The formulas do not give an exact fit, but the results are nevertheless very good. For this linear fit there are several results which are independent of the values of the parameters b and X. For

TABLE I. Excitation energies in MeV of single analog (SA) (half integer T) states and double analog (DA) states in the *f-p* shell.

$T=0$	^{44}Ti (9.340), ^{48}Cr (8.75), ^{52}Fe (8.559)
$T=1/2$	^{43}Sc (4.274) [a], ^{43}Ti (4.338) [a], ^{45}Ti (4.176), ^{49}Cr (4.49), ^{51}Mn (4.451), ^{53}Co (4.390), ^{53}Fe (4.250)
$T=1$	^{46}Ti (14.153), ^{50}Cr (13.222)
$T=3/2$	^{45}Sc (6.752) [a], ^{47}Ti (7.187), ^{51}Cr (6.611)
$T=5/2$	^{47}Sc (8.487) [a], ^{49}Ti (8.724)

[a]Obtained from binding-energy data.

TABLE II. The calculated excitation energies of single analog ($J=j$) states (SA) and double analog ($J=0^+$) states (DA). A comparison is made of single *j*-shell calculations using the spectrum of ^{42}Sc as input and linear fits.

Single analog	Single *j* MeV	$b(T+X)$ [a] MeV	Formula
^{43}Ti (^{53}Co) [b]	4.142	4.176	$b(0.5+X)$
^{45}Ti (^{51}Mn)	4.112	4.176	$b(0.5+X)$
^{45}Sc (^{51}Cr)	6.601	6.496	$b(1.5+X)$
^{47}Ti (^{49}V)	6.590	6.496	$b(1.5+X)$
^{49}Ti (^{47}Sc)	8.829	8.816	$b(2.5+X)$
Double analog		$2b(T+X+1/2)$ [a]	
^{44}Ti (^{52}Fe)	8.284	8.352	$2b(0.5+X)$
^{48}Cr	8.000	8.352	$2b(0.5+X)$
^{46}Ti (^{50}Cr)	13.204	12.992	$2b(1.5+X)$
^{48}Ti	17.659	17.632	$2b(2.5+X)$

[a] $b=2.32$ MeV, $X=1.30$, $T=|N-Z|/2$.
[b] Also the mirror nuclei ^{43}Sc (^{53}Fe).

example, states with the same T should have the same SA excitation energies. This is not strictly true in the single *j*-shell model. However, the single *j*-shell results are very close for ^{43}Ti and ^{45}Ti, 4.142 and 4.112 MeV, respectively. The difference is only 30 keV. Wherever the single *j* shell gives a two to one ratio for the energies of DA states as compared with SA states so does the linear fit, irrespective of what *b* and *X* are.

The single *j*-shell calculations yield two to one ratios of DA to SA for the pairs (^{44}Ti,^{43}Ti), (^{44}Ti,^{43}Sc), (^{48}Ti,^{49}Ti) and (^{48}Ti,^{47}Sc), (^{52}Fe,^{53}Fe) and so also do the linear formulas. But the linear formulas also give two to one ratios where the single *j* shell does not. These include (^{46}Ti,^{45}Sc) and (^{46}Ti,^{47}Ti). In the single *j* shell the excitation energies are 13.204 MeV for ^{46}Ti and 6.590 MeV for ^{47}Ti yielding a ratio of 2.0036.

The (^{46}Ti,^{45}Sc) case was considered by Zamick and Devi [2]. They noted that if in the single *j*-shell calculation one neglected the seniority-four admixtures, then one would get a two to one relation because then the dimensions of the basis states would be the same — four (in the exact case they were six for ^{46}Ti and seven for ^{45}Sc). Indeed in the 4×4 diagonalization there will be a two to one relation for *all* the states, not just the analog state and as mentioned in Ref. [2] even if one does not neglect seniority−four states one can see an approximate correction between the energies and wave functions of several of the states in the two nuclei.

However, the case (^{46}Ti,^{47}Ti) is different. There are 17 $J=j$ basis states for ^{47}Ti, but as previously mentioned, only six for ^{46}Ti. Nevertheless the DA analog excitation energy in the single *j*-shell calculation is very close to twice that of the SA excitation energy in ^{47}Ti. The actual ratio is 2.0036.

Note also in Table II that the calculated SA states in ^{45}Sc and ^{47}Ti have nearly the same excitation energies (6.601 and 6.590 MeV). Again the configurations look completely different. In ^{45}Sc we have one proton and four neutrons. The four neutrons could have seniority 0, 2, or 4. In ^{47}Ti we have two protons and three neutron holes. The only common thread between the two nuclei is that they have the same neutron excess $N-Z=3$. Indeed the linear approximation yields both the two to one relation between the DA in ^{46}Ti and the SA in ^{47}Ti and and the equality of the SA excitation energies of ^{45}Sc and ^{47}Ti.

We now focus on the *experimental* results in Table I. We start with relations which are in theory at least the most exact and as we go down the list the number of approximations increase. We will see that agreement with experiment does not necessarily follow in the same order. First we discuss *mirror nuclei* where we expect the excitation energies to be the same as long as one neglects charge symmtery-breaking interactions, especially the Coulomb interaction. For the mirror pair (^{43}Sc,^{43}Ti) the *experimental* excitation energies are 4.274 and 4.338 MeV; for the pair (^{53}Fe,^{53}Co) the values are 4.250 and 4.390 MeV.

Next there are relations that are *exact* in the single *j*-shell approximation but not when configuration mixing is present. First in this category are the cross conjugate relations [1]. The cross conjugate of a given nucleus is one in which the protons are replaced by neutron holes and the neutrons by proton holes. In the single *j* shell the spectrum of cross conjugate pairs should be the same. The pairs and their experimental excitation energies in MeV are (^{44}Ti,^{52}Fe) (9.340,8.559), (^{43}Sc,^{53}Fe) (4.274,4.250), (^{43}Ti,^{53}Co) (4.338,4.390) and (^{47}Sc,^{49}Ti) (8.487,8.724). Except for the first case (^{44}Ti,^{53}Fe) the cross conjugate relations are well satisfied.

Next we consider other less obvious two to one relations which are exact in the single *j*-shell approximation. In order to make the comparison easy we give the experimental energy of the even-even nucleus and twice the energy of the odd *A* nucleus. For (^{44}Ti,^{43}Ti) the excitation energies in MeV are (9.340,8.558) and for (^{52}Fe,^{53}Fe) they are (8.559,8.500). Again, as in the cross conjugate case ^{44}Ti presents a problem. We will soon consider configuration mixing calculations to see if this problem can be resolved.

We then consider experimental results for cases in which there are *approximate* two to one relations for *all* levels in the single *j*-shell approximation which would be exact if seniority-four admixtures are neglected. There is a visual approximate similarity of the numbers in the column vectors describing the even-even and even-odd systems [2]. These include (^{46}Ti,^{45}Sc) (14.153,13.504) and (^{50}Cr,^{51}Cr) (13.222, 13.222). Looking back at all the experimental data above it would appear that the single *j*-shell approximation works much better in the upper half of the $f_{7/2}$ region than in the lower half.

We next consider cases in which the single *j*-shell approximation does not obviously yield the exact or approximate (in the sense of ^{45}Sc, ^{46}Ti) relations between the excitation energies of different nuclei, but the linear approximation does. Consider first the $T=0$ states in Table I. Whereas by cross conjugate symmetry ^{44}Ti and ^{52}Fe should have the same excitation energies there is no such prediction for ^{48}Cr. The excitation energy of ^{48}Cr is 8.75 MeV, not too far away from the value of ^{52}Fe of 8.559 MeV.

TABLE III. Single j and configuration mixing calculations (CMC) with the FPD6 interaction.

	Single j A dependent MeV	Single j A independent MeV	CMC A dependent MeV
^{43}Ti	3.089	3.115	4.246
^{44}Ti	6.129	6.230	9.290
^{45}Sc	4.875	4.993	6.556
^{45}Ti	3.047	3.122	4.759
^{46}Ti	9.676	9.890	13.796
^{50}Cr	9.397	9.989	11.398 [a]
^{51}Cr	4.666	4.994	5.768 [a]
^{52}Fe	5.781	6.230	7.050 [a]
^{53}Fe	2.872	3.115	3.548 [a]

[a]Only two particles were excited.

For $T=1/2$ the energies for the seven cases range from 4.176 to 4.451 MeV. The excitation energies are reasonably constant. There is no obvious relation in the single j-shell between ^{43}Ti and ^{45}Ti (the dimensions of the matrices are 4 and 17, respectively, but the energies are reasonably close 4.338 and 4.176 MeV, respectively). For $T=3/2$ there is no obvious relation between ^{45}Sc and ^{47}Ti but the energies are again reasonably close 6.752 and 7.187 MeV.

In Table III we show the effects of configuration mixing by doing both single j and full fp calculations with the FPD6 [4] interaction for some nuclei. It should be noted that in the OXBASH program [5] that we use the FPD6 interaction matrix elements and single particle energies vary as $A^{-0.35}$. We present the results with this A dependence. In the single j-shell case we also show results for fixed A ($A=42$) in order to show the various symmetries which are also present in Table II. [Note that since all the input scales as $A^{-0.35}$, so also do the excitation energies in the first and last column of Table III].

Note that the single j excitation energies here are lower than the single j calculations which use matrix elements from experiment. However, in the full f-p calculation these energies become larger. If we compare ^{43}Ti and ^{44}Ti we see that in the single j shell with the A-independent interaction the SA analog excitation in ^{44}Ti is exactly twice that of ^{43}Ti, as of course it must be. In the full f-p shell calculation the calculated DA energy in ^{44}Ti (9.290 MeV) is more than twice the SA energy in ^{43}Ti (8.492 MeV) and is therefore in qualitative agreement with experiment. There is a similar story for the pair ^{45}Sc, ^{46}Ti where an *approximate* two to one relation should hold in the single j shell and indeed twice the ^{45}Sc energy A-independent 9.986 MeV is very close to the ^{46}Ti energy 9.890 MeV. With configuration mixing there is a larger deviation (13.112 MeV vs 13.796 MeV) and the results are closer to experiment. For the cross conjugate partners of ^{46}Ti and ^{45}Sc namely, ^{50}Cr and ^{51}Cr we were only able to perform calculations in which up to two particles were excited from the $f_{7/2}$ shell to the rest of the f-p shell. The calculated values are 11.398 and 11.536 MeV for the DA excitation energy in ^{50}Cr and twice the SA excitation energy in ^{51}Cr. Likewise in ^{52}Fe and ^{53}Fe only two particles are excited. The corresponding energies are 7.050 and 7.096 MeV. The difference is much less than for ^{44}Ti and ^{43}Ti.

We next compare ^{45}Ti and ^{43}Ti, for which in the single j shell there is no obvious relationship. Nevertheless, the calculated results are very close in the single j A-independent case 3.122 and 3.115 MeV, respectively, only a 7 keV difference. It is not clear why the numbers are *so* close except for the common feature that the value of $|N-Z|$ is the same for both nuclei. However, there are departures from this result in configuration mixing.

Last it should be re-emphasized that the single j-shell results agree much better with experiment in the upper half of the $f_{7/2}$ shell than in the lower part. We already mentioned the nearly exact two to one relation for ^{50}Cr and ^{51}Cr. Also impressive are the experimental results for ^{52}Fe and ^{53}Fe, 8.559 and 4.250 MeV, respectively.

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