Perturbation of linearly transformed energy spectra by configuration mixing

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We study the effect of configuration mixing on the well known linear relations between the energy spectra of j^2 and j^n configurations. We show that both single-particle excitations and third-order corrections lead to breakdown of these relations. Contributions from the former tend to cancel when many high-lying orbits contribute simultaneously.

[NUCLEAR STRUCTURE Linear relations between leads, configuration mixing effects.]

I. INTRODUCTION

Theoretical linear relations between the energy spectra of pairs of simple configurations such as $j^2 \to j^n$ and $j_1 j_2 \to j_1 j_2^{-1}$ have been well known for some time[1,2] and are of considerable interest not only because of their direct connection with the effective two-body interaction[3] but also because of the implications with respect to nuclear structure. For instance, relatively recent work on the experimental spectra of (^{50}Ti, ^{51}V),[4] (^{92}Mo, ^{93}Tc),[5] and (^{210}Po, ^{211}At) (Ref. 6) shows that these pairs all follow the theoretical $j^2 \to j^3$ relationships (where the levels have been appropriately identified) with a remarkable fidelity, suggesting that the structures of j^2 and j^3 should be good approximations for these nuclei. On the other hand, the experimental data[3] for the spectral pairs (^{38}Cl, ^{40}K), (^{42}Sc, ^{48}Sc), (^{48}Sc, ^{54}Co), and (^{92}Nb, ^{96}Nb) satisfy the $j_p j_n \to j_p j_n^{-1}$ (Pandya) transformation with variable and questionable success. In the apparent best of these four cases, namely, the well-known pair (^{38}Cl, ^{40}K), the three, relative, two-body matrix elements that can be extracted from the energy levels are shown in Table I together with the experimental values given in Ref. 3. Also shown are the parameters of the local equivalent of the Kallio-Kolltveit potential[7] derived in Ref. 8 [the Petrovich, McManus, Madsen (PMM) potential]. The particularly poor correspondence between the (^{38}Cl, ^{40}K) difference for the (3^-–5^-) matrix elements and the other entries underscores the fact that the success of the linear relations in relating certain spectral pairs may have little significance in the prediction of spectra (or other properties) in other nuclei.

TABLE I. Relative two-body matrix elements for $(\pi d_{3/2})$ $(\nu f_{7/2})$, extracted from the energy levels of (^{38}Cl, ^{40}K), and their difference values.

Spin pairs	Difference values between spin pairs: Exptl spectrum[a]	Exptl (Ref. 3)	PMM[b]
$4^-,3^-$	0.55	0.45	0.50
$3^-,5^-$	0.09	0.35	0.38
$5^-,2^-$	0.67	0.65	0.67

[a] Derived from (^{38}Cl, ^{40}K) experimental spectrum.
[b] From the PMM potential (see Ref. 8).

In this paper we do not propose a particular answer to the (^{38}Cl, ^{40}K) problem, which does not appear amenable to any simple explanation (see Sec. VI). Instead we will enlarge on the approach first given by Talmi[1] and treated in detail in Ref. 2. In sum, as shown in these references, the second-order effects due to configuration mixing from a certain type of two-particle excitation can be renormalized in the two-body interaction. For the purposes of our discussion, we express this as follows: We assume the first-order interaction energies are related by

$$E(j^n)_J = \sum_{J'} C_{J'} E(j^2)_{J'} \,. \tag{1}$$

We define the second-order perturbation effects by

$$\Delta E(j^n)_J = {\sum_{j'j''}}' \Delta E(j^n \to j^{n-2} j' j'')_J \,, \tag{2}$$

$$\Delta E(j^2)_{J'} = {\sum_{j'j''}}' \Delta E(j^2 \to j' j'')_{J'} \,, \tag{3}$$

where the primes on the summation symbols signify the exclusion of the term corresponding to $j' = j'' = j$. Then it is true[1,2] that

$$\Delta E(j^n \to j^{n-2}(j')^2)_J = \sum_{J'} C_{J'} \Delta E(j^2 \to (j')^2)_{J'} \,, \tag{4}$$

where we have suppressed the suffixes n and J in the linear transformation coefficient $C_{J'}$. In general, the equivalence of Eqs. (1) and (4) does *not* hold for third- or higher-order excitations or single-particle excitations of the type $j^2 \to j' j''$ $(j' \neq j'')$ in *any* order, as we shall show in several cases.

The effect of single-particle excitations on the linear relations amongst particle-particle, particle-hole, and hole-hole spectra was studied by Goode, Koltun, and West.[9] In particular, they derived a "triptych" relation involving all three types of spectra, which to first-order is *not* affected by single-particle excitations. Because of our particular interest in observable and possibly predictable effects resulting from single-particle excitations, amongst other breakdown phenomena, we adopt a different approach. We consider five simple examples of configuration mixing and explicitly study the breakdown owing to single-particle excitations and higher-order excitation (> second order). These examples are

(a) Two and four identical particles in a $j=\frac{5}{2}$ subshell perturbed by a $j=\frac{1}{2}$ subshell. In the absence of configuration mixing, four particles in a $j=\frac{5}{2}$ subshell are in a two-hole configuration. When the special case of a pairing interaction is considered, we show explicitly that the linear relations hold *only* up to second order in the interaction.

(b) Three identical particles in a $j=\frac{5}{2}$ subshell perturbed by a $j=\frac{1}{2}$ subshell.

(c) Three identical particles in an $h_{9/2}$ subshell perturbed by a low-lying $f_{7/2}$ subshell. Here, single particle excitations appreciably disturb the linear relations only for the level with $J=j-1=\frac{7}{2}$.

(d) Three identical particles in a subshell j perturbed by *several* other subshells. We find that the linear relations are appreciably perturbed by single-particle excitations involving *individual*, excited-single-particle orbits j'. But if we have *several* nearly degenerate excited-single-particle orbits with a large range of angular momenta, such as all the single particle states in an excited oscillator shell, we find that the single-particle contributions to the deviations from the linear relationships tend to cancel out. We think this result might have relevance in explaining why the shell model works as well as it does.

(e) Six nonidentical particles in a $j=\frac{5}{2}$ subshell perturbed by a $j=\frac{1}{2}$ subshell. If there is no configuration mixing, then this state is a particle-hole configuration of the type $(\frac{5}{2})^n(\frac{5}{2})^{-n}$, $n=1, 2, 3$. Here we consider only $n=1$ $(T=2)$.

Our numerical calculations are made mainly with a surface delta interaction (SDI), but our main conclusion that the breakdown of the linear transformations is generally relatively minor seems to hold for more realistic interactions as well.

II. $(\frac{5}{2})^{2\text{ and }4}$ CONFIGURATION OF IDENTICAL PARTICLES PERTURBED BY A $j=\frac{1}{2}$ LEVEL

For the two particle case, we begin with the following assumption regarding the single-particle energies,

$$\epsilon_{1/2}-\epsilon_{5/2}=\epsilon>0, \tag{5}$$

and also define

$$V_J\equiv\langle(\tfrac{5}{2})^2_J|V|(\tfrac{5}{2})^2_J\rangle, \tag{6}$$

$$W_0\equiv\langle(\tfrac{5}{2})^2_0|V|(\tfrac{1}{2})^2_0\rangle, \tag{7}$$

$$W_2\equiv\langle(\tfrac{5}{2})^2_2|V|(\tfrac{5}{2},\tfrac{1}{2})_2\rangle. \tag{8}$$

Then, up to second order, the energies of the lowest two-particle states $J=0$, 2, and 4, are given by

$$E_0^{(2)}=V_0-W_0^2/2\epsilon, \tag{9}$$

$$E_2^{(2)}=V_2-W_2^2/\epsilon, \tag{10}$$

$$E_2^{(4)}=V_4, \tag{11}$$

and the excitation spectra are given by

$$E_2^{(2)}-E_0^{(2)}=V_2-V_0+W_0^2/2\epsilon-W_2^2/\epsilon, \tag{12}$$

$$E_4^{(2)}-E_0^{(2)}=V_4-V_0+W_0^2/2\epsilon. \tag{13}$$

We consider now the four-particle configuration. Using fractional parentage techniques,[10] it can be shown that the excitation spectrum relative to the $J=0$ ground state is

$$E_2^{(4)}-E_0^{(4)}=V_2-V_0+(W_0^2/2\epsilon)-\tfrac{39}{14}(W_2^2/\epsilon), \tag{14}$$

$$E_4^{(4)}-E_0^{(4)}=V_4-V_0+W_0^2/2\epsilon. \tag{15}$$

Thus the *excitation spectra* satisfy, for example,

$$E_2^{(4)}-E_0^{(4)}=E_2^{(2)}-E_0^{(2)}-\tfrac{25}{14}(W_2^2/\epsilon); \tag{16}$$

and, as expected, the two-particle excitations (i.e., the W_0 term) do not change the excitation spectrum, but one-particle excitations change the $J=0$ to $J=2$ spacing.

Let us now consider a pairing interaction, which, in second order gives rise only to two-particle excitations. We take the same orbitals and occupancies as above, i.e., 2 and 4, identical nucleons in nondegenerate $j=\frac{5}{2}$ and $j=\frac{1}{2}$ orbits. We take the latter orbit an energy ϵ higher and use an attractive SDI of strength G. For two identical particles, the lowest $j=0$ state is at an energy

$$E_0^{(2)}=\epsilon-2G-[(\epsilon+G)^2+3G^2]^{1/2} \tag{17}$$

while the $J=4$ state is at

$$E_4^{(2)}=0. \tag{18}$$

For four identical particles, we obtain

$$E_0^{(4)}=\epsilon-4G-(\epsilon^2+4G^2)^{1/2}, \tag{19}$$

$$E_4^{(4)}=\epsilon-G-(\epsilon^2+G^2)^{1/2}. \tag{20}$$

The excitation energy of the $J=4$ can be expanded in powers of G/ϵ. We find, for the two-particle case that

$$E_4^{(2)}-E_0^{(2)}=3G+\tfrac{3}{2}G^2/\epsilon-\tfrac{3}{2}G^3/\epsilon^2, \tag{21}$$

while for the four-particle case, a similar expansion yields

$$E_4^{(4)} - E_0^{(4)} = 3G + \tfrac{3}{2}G^2/\epsilon + 0G^3/\epsilon^2 \ , \tag{22}$$

both up to order G^3. We see that beyond order G^2 the spectra are different. Yet, in the *strong* coupling limit, $\epsilon = 0$ (where the perturbation expansion naturally breaks down), we obtain again the same excitation energy, this time $4G$, for two and four identical particles. This is a rigorous result for eigenstates of generalized seniority, as is the case for the SDI.[11] Such a result for the degenerate $(G=0)$ case seems to hold even for more general interactions, which give rise to one-particle excitations as well, provided only that the wave functions are eigenstates of the generalized seniority.[11] Here we have investigated the energies for two and four identical particles for an SDI of strength $G = 1$ MeV.

Table II shows the excitation energies for $J=2$ and $J=4$ states for $\epsilon=0$ and 2 MeV and also in the limit $\epsilon \to \infty$. The excitation spectra are seen to be identical in both extreme limits, $\epsilon=0$ and ∞, and do not differ substantially for a typical intermediate case $\epsilon = 2$ MeV.

We may also estimate the four-particle energies by assuming the second-order perturbation results hold exactly. This gives

$$E_2^{(4)} - E_0^{(4)} = E_2^{(2)} - E_0^{(2)} + \tfrac{25}{14}\Delta E_2^{(2)} \ , \tag{23}$$

$$E_4^{(4)} - E_0^{(4)} = E_4^{(2)} - E_0^{(2)} \ , \tag{24}$$

where

$$\Delta E_2^{(2)} \equiv - W_2^2/G \ , \tag{25}$$

which is the second-order energy shift in the $J=2$ state. This is exact for large ϵ. On the other hand, for $\epsilon=0$, the total energy shift for $J=2$ is -1.2 MeV. If we assume that the total energy shift has obeyed Eq. (23), there should be a correction ~-2.14 MeV. Actually there is no correction, which is a symptom of the breakdown of perturbation theory.

TABLE II. Excitation energies (MeV) for two and four identical nucleons in $j=\frac{5}{2}$ subshell perturbed by a $j=\frac{1}{2}$ subshell, using surface δ interaction of strength $G=1$ MeV.

Nucleons	$\epsilon = 0$	$\epsilon = \epsilon_{1/2} - \epsilon_{5/2}$ $\epsilon = 2$	$\epsilon \to \infty$
$E_2^{(2)} - E_0^{(2)}$	2.114	2.349	$2.314 + 0.677/\epsilon$
$E_4^{(2)} - E_0^{(2)}$	3.714	3.178	$2.714 + 1.5/\epsilon$
$E_2^{(4)} - E_0^{(4)}$	2.114	2.201	$2.314 - 0.792/\epsilon$
$E_4^{(4)} - E_0^{(4)}$	3.714	3.277	$2.714 + 1.5/\epsilon$

III. $(\frac{5}{2})^3$ CONFIGURATION OF IDENTICAL PARTICLES PERTURBED BY $j=\frac{1}{2}$ SUBSHELL

For a pure $(\frac{5}{2})^3$ configuration of identical particles, the possible J values are $\frac{3}{2}$, $\frac{5}{2}$, and $\frac{9}{2}$. The energies of these states are well-known linear combinations of the two-particle $J=0$, 2, and 4 energies. Relative to the $\frac{5}{2}$ state, we have

$$E_{3/2}^{(3)} = -\tfrac{2}{3}V_0 + \tfrac{55}{42}V_2 - \tfrac{9}{14}V_4 \ , \tag{26}$$

$$E_{9/2}^{(3)} = -\tfrac{2}{3}V_0 - \tfrac{4}{21}V_2 + \tfrac{6}{7}V_4 \ . \tag{27}$$

We now consider the effect of configuration mixing due to a $j=\frac{1}{2}$ subshell. Table III shows the excitation energies, $\epsilon = 0$, 2, and ∞, of the lowest $(\frac{5}{2}, \frac{1}{2})^3$ states for an SDI of strength $G=1$. The energies obtained by using Eqs. 26, and 27, with the V_J set equal to the exact two-particle energies, are shown in parentheses. As can be seen, the results agree fairly well over the whole range of ϵ.

IV. $(h_{9/2})^{2,3}$ CONFIGURATIONS WITH $f_{7/2}$ ADMIXTURE

Our next example involves some of the configurations in the Pb region. Consider the $N=126$ isotopes, $^{209}_{83}$Bi, $^{210}_{84}$Pb, and $^{211}_{85}$At. The two lowest single-particle states are $0h_{9/2}$ and $1f_{7/2}$. The low-lying two- and three-particle levels were calcu-

TABLE III. Excitation energies (MeV) for three identical particles in $j=\frac{5}{2}$ subshell. Numbers in parentheses are excitation energies obtained by applying the linear relations of Eqs. (26) and (27) to the calculated two-particle energies shown in Table II.

Nucleons	$\epsilon = 0$	$\epsilon = \epsilon_{1/2} - \epsilon_{5/2}$ $\epsilon = 2$	$\epsilon \to \infty$
$E_{3/2}^{(3)} - E_{5/2}^{(3)}$	0.440(0.381)	0.713(1.031)	$1.286 - 1.008/\epsilon$ $(1.286 - 0.77/\epsilon)$
$E_{9/2}^{(3)} - E_{5/2}^{(3)}$	2.768(2.781)	2.256(2.277)	$1.886 + 1.255/\epsilon$ $(1.886 + 1.157/\epsilon)$

lated by Golin[12] for several different interactions including configuration mixing. In the absence of configuration mixing, i.e., pure $(h_{9/2})^3$, the three-particle energies are linear combinations of the two-particle energies, regardless of the form of the interaction. We want to know to what extent these relations still hold in the presence of configuration mixing from the $f_{7/2}$ subshell. The results are shown in Tables IV and V. Here the two-particle excitation energies and the three-particle energies obtained by exact diagonalization are listed and compared with the values obtained by applying the linear relations to the two-particle energies. As seen, the linear relations hold very well for all J values except one, $J=\frac{7}{2}$. This is partially due to the fact that configuration mixing acts mainly in the $J=0$ state, i.e., two-particle excitations. For these, the linear relations hold exactly, up to second order in the interaction. One-particle excitations are indeed rather small for the SDI, which is our test interaction. Only for $J=j-1=\frac{7}{2}$, which is the first excited state, do the linear relations fail significantly, presumably because the one-particle excitations are most important in this state. It is interesting that for the analogous case of $(j=\frac{5}{2})^3$ shown in Table III, the linear relations work much better for $J=\frac{9}{2}$ than for $J=j-1=\frac{3}{2}$. Golin[12] also considers two other interactions, those reported by Kuo-Brown[13] and Schiffer-True,[3] with similar results. The same situation applies to the neutron configurations ^{209}Pb, ^{210}Pb, and ^{211}Pb where the two lowest single-particle states are, respectively, $g_{9/2}$ and $i_{11/2}$.

V. THREE IDENTICAL PARTICLES IN A SUBSHELL PERTURBED BY *SEVERAL* OTHER SUBSHELLS

We have not been able to obtain a general relations between the second-order energy shift of two-particle and $(n\geq 3)$ particle configurations arising from *one*-particle excitations. However, we are able to obtain an approximate sum rule in one special case: the interaction energy for a (j^3) configuration of identical particles. For this case, Eq. (1) yields for the first-order interaction energy,

$$E(j^3)_J=\sum_{J'} C_{J'}E(j^2)_{J'}\,, \tag{28}$$

where, as before, the C_J coefficient is proportional to the square of the fractional parentage coefficient.

Next, consider the second-order perturbation contribution to the energy arising from one-particle excitations. For the two-particle case, we have

$$\Delta E(j^2\to jj')_J=-\frac{\langle (jj')_J|V|(j^2)_J\rangle^2}{\epsilon}\,, \tag{29}$$

as a result of excitation of a nucleon from j to j'.

For the three-particle case, we can show by using the formulas given by de Shalit and Talmi[10] that

$$\Delta E(j^3\to j^2j')_J=\sum_{J'} C_{J'}S_{j'J'J}\Delta E(j^2\to jj')_{J'}\,, \tag{30}$$

where

$$S_{j'J'J}=2(2J'+1)\sum_{J_1\,\text{even}}(2J+1)\begin{Bmatrix} 2 & 2 & J_1\\ j' & J & J'\end{Bmatrix}^2 . \tag{31}$$

{Actually to obtain this result, we have dropped cross terms proportional to

$$[\Delta E(j^2\to jj')_{J'}\Delta E(j^2\to jj')_{J''}]^{1/2}\,,$$

with $J''\neq J'$}.

According to Eq. (30) if all S coefficients were equal to unity, second-order corrections to the energy resulting from one-particle excitation would follow the *same* linear relations as the first-order energies, as also occurs for two-particle excitations. However, this is not generally the case. First of all, if the sum in Eq. (31) were over *all*

TABLE IV. Excitation energies (MeV) for $(h_{9/2},f_{7/2})$ subshell of $^{210}_{84}$Po and $^{211}_{85}$At, using surface delta interaction of strength $4\pi G=0.0092$ MeV.

	$\epsilon(f_{7/2})-\epsilon(h_{9/2})=0.897$ MeV (from Ref. 12)	
J	$(h_{9/2})^2$	$(h_{9/2},f_{7/2})^2$
0	−0.80	−1.03
2	−0.19	−0.21
4	−0.10	−0.11
6	−0.06	−0.07
8	−0.03	−0.04

TABLE V. Excitation energies (MeV) for $(h_{9/2},f_{7/2})^3$ subshell of $^{210}_{84}$Po and $^{211}_{85}$At relative to $J=\frac{9}{2}$ ground state (see Ref. 12). Values obtained from $(h_{9/2},f_{7/2})^2$ energies by applying linear relations are given for comparison.

J	Experimental	From linear relations
$\frac{3}{2}$	0.72	0.71
$\frac{5}{2}$	0.67	0.66
$\frac{7}{2}$	0.60	0.69
$\frac{9}{2}$	0.73	0.74
$\frac{11}{2}$	0.70	0.70
$\frac{13}{2}$	0.69	0.69
$\frac{15}{2}$	0.80	0.81
$\frac{17}{2}$	0.80	0.81
$\frac{21}{2}$	0.85	0.86

J_1 states and if the nucleons were identical, we would obtain

$$S_{j'J'J}=2\ , \tag{32}$$

so the second-order correction would be twice as large as required for the same linear relations to hold as for the first-order energies. Actually, of course, a (j^2) configuration of identical particles can have only *even* J_1. Thus if we calculate S for the specific configuration already considered in this paper, namely, $j=\frac{5}{2}$ and $j'=\frac{1}{2}$, J' can only equal 2, and we find

$$\begin{aligned} &S_{1/2,2,3/2}=\tfrac{4}{3}\ ,\\ &S_{1/2,2,5/2}=\tfrac{1}{2}\ ,\\ &S_{1/2,2,9/2}=\tfrac{1}{6}\ . \end{aligned} \tag{33}$$

We see again that the second-order energies for the three-particle case do not follow the same linear relation as the first-order energies. However, suppose we have several excited single-particle states j', in fact *all* values of j' from $(j-J')$ to $(j+J')$, and all with the same single-particle excitation energy. In this case, using the SDI, it is readily shown that

$$\Delta E(j^2\to jj')_J=\phi(j,J)(2j'+1)(j\tfrac{1}{2}j'-\tfrac{1}{2}J0)^2\ , \tag{34}$$

where the detailed form of $\phi(j,J)$ is not of direct concern here. The dependence on j' is given by Eq. (34). For the three-particle case, we write

$$\Big(\sum_{j'}\Delta E(j^3\to j^2j')\Big)_J =\sum_{J'}C_{J'}\sum_{j'}S_{j'J'J}\Delta E(j^2\to jj')_{J'}\ , \tag{35}$$

where we have summed over particle states j'. Now we define $\overline{S}(J',J)$,

$$\overline{S}(J',J)\equiv\frac{\sum_{j'}S_{j'J'J}\Delta E(j^2\to jj')_{J'}}{\sum_{J'}\Delta E(j^2\to jj')_{J'}}\ , \tag{36}$$

which, it turns out, is independent of $\phi(j,J)$ [see Eq. (34)].

For the linear relationships to hold exactly would require that $\overline{S}(J',J)=1$ for all possible (J',J) values. As might be expected, this is not the case. However, the deviation of $\overline{S}(J',J)$ from unity is small enough so that the linear relationships are not appreciably affected. We illustrate this for $j=\frac{5}{2}$, where, for $(\frac{5}{2})^3$, $J=\frac{3}{2},\frac{5}{2},\frac{9}{2}$ and $J'=0, 2, 3$. The relevant values of $\overline{S}(J',J)$ are given in Table VI. The mean value of $S(J',J)$ for this case is 0.8 and the rms variance is 0.10. If, for the sake of the present argument, we limit ourselves to second-order excitations of the type $(j)^2\to(j')^2$ and $(j)^2\to(j,j')$ but allow *all* possible values of j', we may write the following linear transformation for the perturbed energies E'_J for the spectrum of j^3:

$$E'_J(d^3)=\sum_{J'}C_{j'J}E(j^2)_{J'}+\sum_{j'}[\,]\ , \tag{37a}$$

$$[\,]\equiv\Delta E(j')^2_{J'}+S(J',J)\sum_{j'}\Delta E(j^2\to jj')_{J'}\ , \tag{37b}$$

where the $C_{J',J}$ are again fractional parentage coefficients. If all $S(J',J)$ were equal to unity, the perturbed energy differences would follow the same rule as given in Eq. (1) but, this time, include all second-order single-particle excitations. Clearly, it is a reasonable presumption that the character of the one-particle excitations to the distant states is such that the linear relations are not significantly violated and thus can be simulated by a renormalization of the effective interaction. As far as second-order one-particle excitations are concerned, we may expect that only *nearby* and fragmentary configurations lead to a significant breakdown of the linear transformations.

VI. PARTICLE-HOLE TRANSFORMATIONS

The best known examples of the particle-hole transformations in the ^{40}Ca to ^{56}Ni region are $({}^{38}_{17}\mathrm{Cl}-{}^{40}_{19}\mathrm{K})$ and ${}^{42}_{21}\mathrm{Sc}-{}^{54}_{27}\mathrm{Co})$.[9] In the first case, the linear relations hold extremely well,[14] and even *better* than expected wtih "reasonable" interactions such as SDI, Kuo-Brown, and Schiffer-True. Although, as already noted, we cannot explain this precisely, perhaps the effects of configuration mixing on the linear relations tend to cancel for the same reasons presented in the last section for the $j^2\to jj'$ transformations.

In the second case (Sc and Co), the linear relations are significantly violated. Using the arguments of Sec. V, this violation can be roughly understood if we have a *single*, low-lying, perturbing $p_{3/2}$ orbit. As a simple example, we will consider the particle-particle and the "particle-hole" configurations, $(\frac{5}{2})^2$ and $\frac{5}{2}(\frac{5}{2})^{-1}$, i.e., in the absence of configuration mixing. The latter configuration involves six particles. (For the analogous case of $f_{7/2}$ and $1p_{3/2}$, we would have $(f_{7/2})^2$, i.e., ^{42}Sc, and $(f_{7/2}f_{7/2}{}^{-1})$, i.e., ^{48}Sc.) For the particle-particle configuration, we will consider isospin states of 1 and 0. In the absence of configuration mixing, the former has $J=0$, 2, and 4 (already considered) and the latter, $J=1$, 3, and 5. For the particle-

TABLE VI. Values of $S(J',J)$ for $j=\frac{5}{2}$.

	$J=\frac{3}{2}$	$J=\frac{5}{2}$	$J=\frac{9}{2}$
$J'=0$	···	0.833	···
$J'=2$	0.929	0.810	0.762
$J'=4$	0.570	0.857	0.843

TABLE VII. Excitation energies (MeV) for six identical nucleons in $j=\frac{5}{2}$ subshell, $T=2$ and 3. The energy differences in parentheses were obtained by using the Pandya relations, see Eq. (45).

Nucleons	$\epsilon=0$	$\epsilon=\epsilon_{1/2}-\epsilon_{5/2}$ $\epsilon=2$	$\epsilon\to\infty$
$E_0^{(6)}-E_4^{(6)}$	2.619(2.998)	3.071(2.945)	$2.714+2.60/\epsilon$ $(2.714+0.10/\epsilon)$

hole case, we have a pure $(\frac{5}{2})^6$ configuration, $J=0$ for $T=3$ and $J=1$, 2, 3, 4, and 5 for $T=2$. States with $T=1$ or 0 cannot correspond to particle-hole configurations.

The de Shalit-Talmi theorem for two-particle excitations holds also for nonidentical particles. Thus the Pandya relations,[14] which connect the energies of $\frac{5}{2}(\frac{5}{2})^{-1}$ and $(\frac{5}{2})^2$, still hold when the second-order shift (of order W^2/ϵ) resulting from two-particle excitations is included. However, as with identical particles, these relations are broken by one-particle excitations.

For the case treated here, the two, off-diagonal, matrix elements that follow are relevant for one-particle excitations:

$$W_2=\langle(\tfrac{5}{2})^2_2|V|(\tfrac{5}{2},\tfrac{1}{2})_2\rangle_{T=1}\ , \tag{38}$$

$$W_3=\langle(\tfrac{5}{2})^2_3|V|(\tfrac{5}{2},\tfrac{1}{2})_3\rangle_{T=0}\ . \tag{39}$$

Then, the second-order shift S, which results from one-particle excitations, for the two-particle configurations are

$$\Delta E_2^{(2)}=-W_2^2/\epsilon\ , \tag{40}$$

$$\Delta E_3^{(2)}=-W_3^2/\epsilon\ , \tag{41}$$

$$\Delta E^{(2)}_{J\neq 2\text{ or }3}=0\ . \tag{42}$$

For the particle-hole, i.e., six-particle case, we calculated only the energies of the $J=0$ ($T=3$) and $J=4$ ($T=2$) cases. The latter corresponds to the $J^\pi=6^+$ ground state of ^{48}Sc and the former to the $J^\pi=0^+$ analog state.

We find the second-order shift that is due to *one*-particle excitations is

$$E_0^{(6)}=0\ , \tag{43}$$

because there is no $[(\frac{5}{2})^5\frac{1}{2}]$ state with $T=3$, $J=0$. We also find by explicit calculation that

$$E_0^{(6)}-\Delta E_4^{(6)}=-\tfrac{25}{14}\Delta E_2^{(2)}-\tfrac{23}{36}\Delta E_3^{(2)}\ . \tag{44}$$

On the other hand, application of the Pandya relations to the two-particle configurations gives

$$P((\Delta E)^2)_0-P(\Delta E^{(2)})_4=\tfrac{5}{4}\Delta E_2^{(2)}-\tfrac{23}{36}\Delta E_3^{(2)}\ . \tag{45}$$

As noted, Eq. (45) also applies in the presence of two-particle excitations. We see that Eqs. (44) and (45) differ only because of the interaction in $J=2$ states. For this reason we have not considered the excitation energy of the $J=3$ state.

Some of our numerical results are shown in Tables IV, V, and VII and bear out the above. Note, however, that the deviation from the Pandya transformed spectrum changes sign between $\epsilon=0$ and $\epsilon=2$. Also, the effect on configuration mixing is seen to increase the $4\to0$ splitting from 2.7 to 3.07 MeV (a little more than 10%). A similar result (not shown) obtains for the (^{42}Sc – ^{48}Sc) case. Here calculations were not made with the SDI but with the more realistic Kuo-Brown (KB)[13] and PMM[8] interactions. With these, the *jj* coupling values for the (6^+-0^+) splitting are, respectively, 4.7 MeV and 6.6 MeV, compared to the experimental value of 6.6 MeV. Configuration mixing owing to $1p_{3/2}$ level increases the splitting by 20% and 10%, respectively. Thus one might expect that an intermediate interaction between KB and PMM would reproduce the splitting results obtained experimentally.

VII. CONCLUSIONS

It has been known for some time that the linear transformations between energy spectra are preserved for configuration mixing that is due to two-particle excitations to the same orbits, at least up to second order in the interaction.[1,2] We have shown that these relations do not hold in higher order or for single-particle excitations. However, we present arguments to show that in the latter case (up to second order) they do hold *approximately* if there is a large range of j' values for excited single-particle states. This is indeed the case for configuration mixing that is due to high-lying levels. Thus the effect of such configuration mixing on energies also can approximately be simulated by a change in the effective interaction.

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[1]I. Talmi, Rev. Mod. Phys. 34, 704 (1962).

[2]A. de-Shalit and H. Feshbach, *Theoretical Nuclear Physics* (Wiley, New York, 1974), Vol. 1, pp. 340–346.

[3]J. P. Schiffer and W. W. True, Rev. Mod. Phys. 48, 191 (1976).

[4]A. R. Poletti, B. A. Brown, D. B. Fossan, P. Gorodetsky, J. J. Kolata, J. W. Olness, and E. K. Warburton, Phys. Rev. C 10, 997 (1974).

[5]B. A. Brown, D. B. Fossan, P. M. S. Lesser, and A. R. Poletti, Phys. Rev. C 13, 1194 (1976).

[6]I. Bergstrom, B. Fant, C. J. Herrlander, P. Thieberges, and K. Wikstrom, Phys. Lett. 32B, 476 (1970).

[7]A. Kallio and K. Kolltveit, Nucl. Phys. 53, 87 (1964).

[8]F. Petrovich, H. McManus, V. A. Madsen, and J. Atkinson, Phys. Rev. Lett. 22, 895 (1969).

[9]B. J. West and D. S. Koltun, Phys. Rev. 187, 1315 (1969). See also P. Goode, D. S. Koltun and B. J. West, Phys. Rev. C 3, 1527 (1971).

[10]A. de-Shalit and I. Talmi, *Nuclear Shell Theory* (Academic, New York, 1963), p. 540.

[11]R. Arvieu and S. A. Moszkowski, Phys. Rev. 145, 830 (1966); A. Plastino, R. Arvieu, and S. A. Moszkowski, Phys. Rev. 145, 837 (1966).

[12]M. Golin, Brookhaven National Laboratory, Report No. BNL-22641, 1977 (unpublished).

[13]T. T. S. Kuo and G. E. Brown, Nucl. Phys. A114, 241 (1968).

[14]S. P. Pandya, Phys. Rev. 103, 956 (1956); S. Goldstein and I. Talmi, *ibid.* 102, 589 (1956).