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A SUGGESTION FOR CHOOSING THE SINGLE-PARTICLE ENERGIES IN DOUBLE CLOSED SHELL NUCLEI

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Abstract:

The single-particle energies in a nucleus of $A \pm 1$ particles as taken from experiment are seen to be shifted when used for the calculation of the $A$ particle system excited states. This shift can be described as a change in the particle-hole gap arising from an isospin-isospin interaction of the excited nucleon with the remaining core of $A - 1$ particles. It lowers the $T = 0$ states of $^{40}$Ca by about 1.5 MeV and by 3.75 MeV in $^{16}$O and raises the $T = 1$ states one third this amount. This shift gives an account of discrepancies which are observed in all existing T.D.A. or R.P.A. calculations of double closed shell nuclei.

A large number of calculations\textsuperscript{1-8} have already been performed on double closed shell nuclei. The spirit of all these works is essentially the same: one chooses a single-particle basis and splits the hamiltonian $\mathcal{H}$ of the
system into two parts; \( H_0 \), which is already diagonal for the particle-hole excitations \( |j'j^{-1}\rangle \) and a residual interaction \( V \). The eigenvalues of \( H_0 \) are generally taken from the experimental data on the neighbouring \( A \pm 1 \) nuclei. The matrix elements \( \langle (j'j^{-1})_{JT} | V | (j'j^{-1})_{JT} \rangle \) have a component diagonal in the projection quantum numbers of the particle and the hole (and thus independent of \( J \)). This component is a correction to the particle-hole energy \( \epsilon_j - \epsilon_{j'} \):

\[
\langle j'm'jm | V | j'm'jm \rangle
\] (1)

schematized by

\[\begin{array}{c}
  j' \\
  j \\
  j \\
  j' \\
\end{array}
\] (2)

In principle, it takes into account the change in the single-particle energy of a nucleon which interacts with a core of \( A - 1 \) nucleus instead of \( A \). In the same way, however, that one gets better results by using experimental single-particle energies rather than Hartree-Fock energies, the contribution (2) should be corrected for higher order processes and replaced by

\[\begin{array}{cccccc}
  j' & j & j' & j & j & j \\
  j' & j & j' & j & j & j \\
  j' & j & j' & j & j & j \\
  j' & j & j' & j & j & j \\
\end{array} + \text{etc...} \] (3)

Except for the first order contribution, the graphs in (3) are not included either in a TDA or in a RPA calculation. (In Ref. 7 the second order was also included, as discussed below).

The potential corresponding to the measured particle energies in the \( A + 1 \) nucleus can be written as
In order to take the correction (3) into account, we propose the replacement of (4) by

$$V_o(r) + 4 \frac{E'_{A-1}}{A} V_1(r)$$

Let us neglect slight changes in the shape or the magnitude of $V_o(r)$ and $V_1(r)$. We assume in addition that the shift in the single-particle energies is proportional to the change in the potential. These approximations are not necessary for realistic calculations, but they are probably quite good. We get therefore

$$\delta E \sim 4 \frac{e_{1/2}}{A} \left\{ \langle A | \frac{2}{T} | A \rangle - \langle A + 1 | \frac{2}{T} | A + 1 \rangle \right\}.$$  

(5)

$|A + 1\rangle$ and $|A\rangle$ are generally taken as

$$|A + 1\rangle = \alpha_{j'm'}^{+} 1/2 \tau' |T_0 T_0\rangle$$

(6)

$$|A\rangle = \sum_{m \tau, m' \tau'} (1/2 \tau' 1/2 - \tau |T_{T_z}^2 \rangle \langle j'm' j - m |J M \rangle$$

$$a_{j'm'}^{+} 1/2 \tau' (-)^{j-m+1/2-\tau} a_{jm} 1/2 \tau |T_0 T_0\rangle$$

(7)

or, when the Pauli Principle forbids the construction of a particle-hole pair of good isospin

$$|A\rangle = \sum_{m \tau, m'} \langle j'm' j - m |J M \rangle a_{j'm'}^{+} 1/2 \tau (-)^{j-m} a_{jm} 1/2-\tau |T_0 T_0\rangle.$$  

(8)
The notations are standard ones (\( T_0 \) is the isospin of the A particle ground state).

In Table I, the shifts \( \Delta \) are given in units of \( \varepsilon_1 / A \) for double closed shell nuclei. The value of \( \varepsilon_1 \) can be obtained from the symmetry energy of a particle in the 2\( p \) 3/2 orbital of \(^{48}\text{Ca}\)

\[
\varepsilon_s = \varepsilon_n + \Delta - \varepsilon_p = 4 T_0 \varepsilon_1 / A
\]  

(\( \varepsilon \) are the single-particle energies and \( \Lambda \) the Coulomb energy). This gives \( \varepsilon_1 \approx 20 \) MeV, that is for the \( T = 0 \) states \( \delta \varepsilon = -1.5 \) MeV in \(^{40}\text{Ca}\) and \( \delta \varepsilon = -3.75 \) MeV in \(^{16}\text{O}\). We could have equivalently considered (3) as producing a shift in the hole energies which leads to the same results.

When the residual interaction is taken into account, one has to correct for the contribution (1) which is included both in \( \delta \varepsilon \) and in the particle-hole matrix elements. This correction is

\[
\tilde{V}_{j'j}^T = \sum_j \frac{2J + 1}{(2j' + 1)(2j + 1)} \langle (j'j^{-1})JT | \mathcal{V} | (j'j^{-1})JT \rangle
\]

The proper way to include it is to subtract \( \tilde{V}_{j'j}^T \) from the matrix element

\[
\langle (j'j^{-1})JT | \mathcal{V} | (j'j^{-1})JT \rangle
\]

before using this latter in a configuration mixing calculation.

A well known discrepancy of the TDA and RPA calculations (as discussed in Refs. 3-5) can be explained by our model: the excitation energies of the \( T = 0 \) unnatural parity states are generally predicted several a MeV too high in \(^{16}\text{O}\) and \(^{40}\text{Ca}\). This is seen in Table II where the results of various calculations for some \( T = 1 \) states and \( T = 0 \) unnatural parity states in \(^{16}\text{O}\) and \(^{40}\text{Ca}\) are
compared with experiments. Since these states are quite accurately described\textsuperscript{3–5} by a single-particle excitation, the shift $\delta \varepsilon$ and the correction (10) can be approximately included by adding the amount $\delta \varepsilon - V_{j',j}^T$ to the calculated excitation energies. These corrections are shown at the left in Table II for the calculations of Ref. 2,4, where a phenomenological interaction is used. Realistic interactions were used in the calculations leading to the results shown at the right in Table II. Estimates of $V_{j',j}^T$ for such forces were used in arriving at the corresponding corrections shown at the extreme right in Table II.

The corrections are seen to give a reasonable account of the discrepancies occurring in the original\textsuperscript{1–8} calculations for $^{16}O$ and $^{40}Ca$, especially for the $T = 0$ unnatural parity states for which the shift $\delta \varepsilon - V_{j',j}^T$ cancels to a large extent the difference between theoretical\textsuperscript{1–8} and experimental\textsuperscript{14} excitation energies. There is however a tendency for the corrected results to underestimate slightly the excitation energy of the $T = 1$ states (but a calculation including configuration mixing has to be done before any definitive conclusion can be drawn on this latter point). Further, in $^{208}Pb$, an unexplained shift of -30 to -90 keV has been noticed by Blomqvist\textsuperscript{13} for both proton or neutron particle-hole centroid energies. This compares very favorably with our prediction (Table I) $\delta \varepsilon = -\varepsilon_1/A \sim -96$ keV. The two main features of our shift—an $A$ dependence, but no $J$ dependence—are therefore seen to be consistent with the experimental data.

Preliminary calculations\textsuperscript{9} show that this shift also explains why the usual\textsuperscript{1–8} microscopic calculations overestimate, as discussed by Gillet and Sanderson,\textsuperscript{4} the Coulomb mixing of $T = 0$ and $T = 1$ states in $^{40}Ca$.

Blomqvist and Kuo\textsuperscript{7} have included the second order diagram of (3) in their calculation. The contribution they call $A_{ph}$ contains however non-diagonal
terms as well as diagonal ones and their calculation is not directly comparable to ours. Clearly, however, their work shows that higher order contributions are needed to cancel somewhat the drastic features they obtain by including the second order diagrams only (this is also discussed in Ref. 12).

A calculation very similar to (5) has been made in Ref. 16) for comparing calculated and experimental single-particle energies of \(^{16}O\) and \(^{40}Ca\).

Other approaches have also been proposed\(^{10,11}\) which reproduce the shift between the \(T = 0\) and \(T = 1\) states in double closed shell nuclei, resulting from empirical observations in parameterizing effective matrix elements. However, none of them\(^{10,11,16}\) provides an adequate explanation for the mechanism leading to the shift so as to lead to a satisfying framework for the study of configuration mixing. In addition, our model has the advantage over the MSDI\(^{11}\) of permitting the use of either realistic or effective interactions. As well as the study of the improvements already described, the changes in the description of the collective states brought in by this model will be interesting. A complete R.P.A. calculation with these shifts included has therefore been undertaken.\(^9\)

We thank R. Trilling and M. Weigel for communicating their results before publication and for useful comments, and L. Zamick for bringing the calculation of Ref. 16) to our attention.
FOOTNOTES AND REFERENCES

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† On leave of absence from CEN SA CLAY, FRANCE.


15. R. Trilling, unpublished results.

Table I. Shifts in the particle-hole gap arising from the isospin-isospin coupling of the excited particle with the remaining core. Except for a core with isospin $T_O = 0$, the state $|j' j'^{-1} j, T = 1 \rangle$ does not have good total isospin and its shift should be considered as the weighted average of the shifts for the components $|T_O \rangle$ and $|T_O + 1 \rangle$ of good isospin.

<table>
<thead>
<tr>
<th>State</th>
<th>Shift</th>
</tr>
</thead>
<tbody>
<tr>
<td>$</td>
<td>j' j'^{-1} j, T = 0 \rangle$</td>
</tr>
<tr>
<td>$</td>
<td>j' j'^{-1} j, T = 1 \rangle$</td>
</tr>
<tr>
<td>$</td>
<td>j' j'^{-1} j, T = \pm 1/2 \rangle$</td>
</tr>
</tbody>
</table>

$^a$Defined in the text.
Table II. Typical results obtained for $T = 1$ and unnatural parity $T = 0$ states of double closed shell nuclei are compared with the shift in the particle-hole gap we propose to include. The corrected values of $E_{th} - E_{exp}$ are obtained by adding the corresponding values of $E_{th} - E_{exp}$ and $\delta \varepsilon - V_{jj'}^T$, shown in the table. The energies are given in MeV.

<table>
<thead>
<tr>
<th>$^{16}_0$</th>
<th>$^{40}_{Ca}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$J^\pi,T$</td>
<td>$E_{exp}^c$</td>
</tr>
<tr>
<td>$2^-,0$</td>
<td>8.88</td>
</tr>
<tr>
<td>$2^-,0$</td>
<td>12.52</td>
</tr>
<tr>
<td>$2^-,0$</td>
<td>13.97</td>
</tr>
<tr>
<td>$2^-,1$</td>
<td>12.96</td>
</tr>
<tr>
<td>$2^-,1$</td>
<td>18.1</td>
</tr>
<tr>
<td>$2^-,1$</td>
<td>19.1</td>
</tr>
<tr>
<td>$J^\pi,T$</td>
<td>$E_{exp}^c$</td>
</tr>
<tr>
<td>$4^-,0$</td>
<td>6.02</td>
</tr>
<tr>
<td>$4^-,0$</td>
<td>5.61</td>
</tr>
<tr>
<td>$2^-,1$</td>
<td>8.47</td>
</tr>
<tr>
<td>$3^-,1$</td>
<td>7.69</td>
</tr>
<tr>
<td>$4^-,1$</td>
<td>7.66</td>
</tr>
<tr>
<td>$5^-,1$</td>
<td>8.54</td>
</tr>
</tbody>
</table>

$^{a}$Refs. 2-8. The initials refer to the various authors.

$^{b}$Calculation referred as HJA by these authors.

$^{c}$Ref. 14.

$^{d}$Typical values of $V_{jj'}^T$ for realistic forces were used to estimate these shifts. $^{15}$

There are: $V_{jj'}^T \approx -0.35 \begin{cases} 16_0 & V_{jj'}^T \approx 0.1 \\ 40_{Ca} & V_{jj'}^T \approx 1.95 \end{cases}$
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