The isovector and isoscalar multiplet yrast energies and isospin non-conserving forces

The isovector and isoscalar multiplet yrast energies and isospin non-conserving forces are defined by:

\[ E^r_J(\bar{r}, T) = E^r_J(\bar{r}, T) - E^r_J(\bar{r} - T), \quad \bar{Z} = \frac{Z_+ + Z_-}{2}. \]  

The observed MEDs are very small (of the order of 10-100 keV), and entirely due to shell effects. Recently, the experimental information on yrast bands has been extended to isospin triplets \([11, 12]\), thus determining new quantities, the TED given by:

\[ TED_J = E_J(\bar{Z} + 1) + E_J(\bar{Z} - 1) - 2E_J(\bar{Z}). \]  

Both measurements are needed to achieve a clear understanding of the interplay between the Coulomb potential \(V_C\), and \(V_B\), the isospin breaking nuclear interaction.

To analyze them, we start by writing the isovector, \(\beta^{(1)}_r\), and isoscalar, \(\beta^{(2)}_r\), contributions to \(V_B\), as linear combinations of two body matrix elements in neutron-proton \((\nu\pi)\) formalism \((r \equiv r_1 r_2 r_3 r_4, \text{where } r_i \text{ is a sub-shell})\):

\[ \beta^{(1)}_r = V^\nu\pi_{Br} - V^\nu\nu_{Br}, \quad \beta^{(2)}_r = V^\nu\pi_{Br} + V^\nu\nu_{Br} - 2V^\nu\pi_{Br}. \]  

The isoscalar contribution \(\beta^{(0)}_r = V^\nu\nu_{Br} + V^\nu\nu_{Br} + V^\nu\pi_{Br}\) is nil in \(V_B\), while for \(V_C\) we have \(\beta^{(0)}_r = \beta^{(1)}_C = \beta^{(2)}_C = V^\nu\pi_{C}.\)

The MEDs are entirely of isovector origin and the first exact shell model calculations in the full \(pf\) shell indicated that \(V_C^{\text{ho}}\), i.e., calculated in the harmonic oscillator (ho) basis fails to give a satisfactory description \([3]\). The way out proposed in this reference consisted in replacing the harmonic oscillator matrix elements \(V^{\text{ho}}_{C_{\text{str}}/2}\) by empirical ones derived from the \(A = 42\) spectrum which are very different. Therefore, it was hard to attribute the replacement to a renormalization of \(V_C\), expected to be small. But it was equally hard to think in terms of CSB precisely because the effect was so large. Nevertheless the ansatz (or variants of it) worked quite well, and subsequent calculations incorporated it \([4, 5]\) leading eventually to (almost) full quantitative agreement \([12]\) for the MED in \(A = 47, 49, 50\) and 51. When the isoscalar TED data came in, it became clear that both charge independence breaking \([4]\) and CSB had to be invoked.

| TABLE I: Coulomb \((V_C)\), isovector (MED-\(V_C \equiv \beta^{(1)}_{f_{7/2}}\)) and isoscalar \((TED-\(V_C \equiv \beta^{(2)}_{f_{7/2}}\)) energies (keV) in \(A = 42\). \(V_C\) calculated in the oscillator basis (ho) |
|-----------------|----|----|----|----|
| \(V_C \equiv V^{\text{ho}}_{C_{\text{str}}/2}\) | 81.60 | 24.60 | 6.40 | -11.40 |
| \(E_J^{[42\text{Ti} - 42\text{Ca}] - V_C}\) | 5.38 | 92.55 | 4.57 | -47.95 |
| \(E_J^{[42\text{Ti} + 42\text{Ca} - 42\text{Sc}] - V_C}\) | 116.76 | 80.76 | 2.83 | -42.15 |

Ironically, this result is obvious from the, long known, \(A = 42\) spectra \([14]\). Assuming that the observed states are essentially \(f_{7/2}^{2}\) configurations on top of the \(40\text{Ca}\) core, these spectra define an interaction in the \(f_{7/2}\) subshell. Therefore, by setting \(V_C \equiv V^{\text{ho}}_{C_{\text{str}}/2}\), the nuclear...
isovector and isotensor contributions can be extracted. They are shown in Table 1, where their centroids — \( \sum_J(2J+1)V_{f\tau/2}^J/\sum_J(2J+1) \)— have been subtracted for clarity. The assumption of \( f_{7/2}^2 \) dominance is not warranted, as—at least— the \( J = 0 \) and \( 2 \) states are known to mix with core excitations. Therefore a safer procedure consists in replacing the lowest observed states by the \( f_{7/2}^2 \) centroids estimated from spectroscopic factors \([4]\). However, when this is done, no significant change obtains in Table 1, whose indications must therefore be taken very seriously.

A renormalized \( V_C \) adapted to the \( f_{7/2}^2 \) space will remain a purely \( \pi\pi \) force, and therefore the same for the isovector and isotensor channels. Furthermore, it is expected to be reasonably close to the bare \( V_C \) in the first line of Table 1. Therefore, upon subtracting this bare \( V_C \) from the observed data—second and third lines—we expect the same, reasonably small numbers. It is obvious that the corresponding numbers are neither equal nor small. The unavoidable conclusion is that the \( A = 42 \) data indicate that the role of isospin non conserving nuclear forces is at least as important as that of the Coulomb potential in the observed MED and TED.

For the full description of these quantities in \( A = 46-51 \) we rely on exact, isospin conserving shell model calculations \([13]\) with single particle spectrum from \(^{41}\)Ca and the KB3G interaction. Very little changes are observed if the other standard interactions are used (KB3, FPD6, all defined in \([14]\)). The energy differences are obtained in first order perturbation theory \([15]\), as the sum of expectation values, in which we separate the monopole and multipole components of the Coulomb field \( V_C = V_{Cm} + V_{CM} \) following Refs. \([16,12]\):

\[
\text{MED}_J = \Delta_M(V_{Cm})_J + \Delta_M(V_{CM})_J + \Delta_M(V_B)_J, \quad (4)
\]

\[
\text{TED}_J = \Delta_T(V_{Cm})_J + \Delta_T(V_B)_J. \quad (5)
\]

The monopole \( V_{Cm} \) contains all terms quadratic in scalar products of Fermion operators \( a_i^\pi \cdot a_j^\pi \). The non diagonal contributions \( i \neq j \) lead to isospin mixing that demands second order perturbation theory. They will be considered here only through their influence on the radial wavefunctions, i.e., the Thomas Ehrman shift that depresses the single particle \( p_{3/2} \) state in \(^{41}\)Sc by \( 200 \) keV below its analogue in \(^{41}\)Ca. The diagonal part \( i = j \) involves only proton number operators. It contains \( E_C \) plus a single particle splitting induced by \( V_C \) on the orbits of principal quantum number \( p \) above harmonic oscillator (ho) closed shell \( Z_{cs} \) \([22]\):

\[
\varepsilon_{Cl} = \frac{-0.001 \ Z_{cs}^{13/12} [2l(l+1) - p(p+3/2)]}{A^{1/3} (p+3/2)} \text{MeV}. \quad (6)
\]

The effect of \( E_C \) is proportional to the difference of (inverse) radii between a \( J \)-yrast and the ground state \([9]\). The total radii depend on those of the individual orbits, and therefore—to good approximation—on the average neutron plus proton occupancies for each orbit, which we denote by \( \langle m_k \rangle /2 \), with \( m_k = z_k + n_k \) (number of neutrons plus number of protons in orbit \( k \)). We take averages relying on the near equality of proton radii in both members of a mirror pair \([9]\). As it is reasonable to assume that orbital radii depend only on \( l \), and the \( p_{1/2} \) occupancy is always negligible, the whole radial effect will be taken to depend on the \( p_{3/2} \) occupancy. Note that the single particle contribution from Eq. (4) is proportional to the difference of proton and neutron occupancies. It is important in \( A = 41 \), but typically ten times smaller than the radial effect in \( A = 47-51 \), so we neglect it and end up with \( \Delta_M(V_{Cm})_J = a_m \langle m_{p_{3/2}} \rangle /2 \). The value of \( a_m \) can be estimated by adding to the observed shift the single particle splitting \([22]\) that depresses the \( l = 3 \) orbits with respect to the \( l = 1 \) ones (by 125 keV at \( A = 40 \), \( Z_{cs} = 20 \)). Then, \( a_m \approx 0.200 + .125 = 0.325 \) MeV.

In the isotensor case the \( m_{p_{3/2}} \) contributions cancel out.

The multipole contribution \( \Delta(V_{CM})_J \) is calculated using oscillator Coulomb matrix elements in the \( pf \) shell. The only direct information on \( V_B \) comes from Table 1.

![FIG. 1: Example of MED renormalization in \( A = 50 \)](image)

To make use of it we must explore the possibility of specifying an interaction acting in the full \( pf \) shell, solely in terms of \( f_{7/2}^2 \) matrix elements. The idea turns out to be quite viable using the multiplicative prescription \([23]\)

\[
\Delta(V_{Cpf}^h) = b \Delta(V_{Cpf}^h)_{J=2}, \quad (7)
\]

as illustrated for the Coulomb potential in Fig. 1.

The same form efficiently relates the schematic pairing or quadrupole pairing forces in the \( pf \) shell to the \( V_{f\tau/2}^{J=0} \) or \( V_{f\tau/2}^{J=2} \) matrix elements. To minimize the number of parameters, for \( V_B \) we retain only the leading term suggested by Table 1, and set \( \beta_{pf}^{(1)} = \beta_1 V_{f\tau/2}^{J=2} \)

\[
\beta_{pf}^{(2)} = \beta_2 V_{f\tau/2}^{J=0}, \quad \text{where } V_{f\tau/2}^{J} \text{ is the matrix element with unit value. Collecting all the pieces we have}
\]
The reduction of $V_B$, for MED and TED, to a single matrix element is an oversimplification, but the results are so satisfactory that the need of extra terms is not felt.

The only parameter-free alternative is to take matrix elements with the weights in Table I. However, this choice is arbitrary because—from the discussion around Eq. (7)—we expect a case by case (even matrix element) renormalization. Nonetheless, though the agreement with experiment becomes less impressive, it remains acceptable. The conclusion is that the leading term in $J = 2$ for MED is indeed dominant, and that in $J = 0$ for TED very dominant.

In Figs. 2 and 3 for the MED, $V_{Cm}$, $V_{CM}$, and $V_{BM}$ stand respectively for the first, second and third terms in Eq. (8). The parameters are taken to be round numbers, $a_m = 300$ keV and $\beta_1 = \beta_2 = 100$ keV.

In Figs. 2 and 3 for $A = 47$ and 49 are quite far from the observed pattern, which is accurately reproduced only after these disparate terms are added. For $A = 50$ and 51 we have replaced the $V_{BM}$ part by a variant of the full sum in which $\beta_1$ is halved. For $A = 50$ the changes are insignificant, but there is a definite improvement in $A = 51$ (remember again Eq. (8) and footnote before it).

It is especially worth noting in Fig. 2 for $A = 49$ and 51 we have replaced the $V_{BM}$ part by a variant of the full sum in which $\beta_1$ is halved. For $A = 50$ the changes are insignificant, but there is a definite improvement in $A = 51$ (remember again Eq. (8) and footnote before it).

The experimental TED patterns in Fig. 3 for $A = 46$ and 50 are quite nicely reproduced by the minimal $\beta_{pf}^{(2)} = \beta_2 V_{fr=0}^{J=0}$ choice. As mentioned, the inclusion of the $J \neq 0$ terms (third line of Table I) makes little difference, and—interestingly enough—simply ignoring $V_B$ and doubling $V_{CM}$ (or the other way round) makes practically no difference. Which confirms the overwhelming dominance of $J = 0$ pairing.

FIG. 2: Experimental and calculated MED for the pairs $^{47}$V–$^{47}$Cr, $^{49}$Cr–$^{49}$Mn, $^{50}$Cr–$^{50}$Fe, and $^{51}$Mn–$^{51}$Fe.

FIG. 3: TED for $A = 46$ and 50
It can be hoped that a rigorous treatment calling upon state of the art CSB potentials \[9,10\] will confirm the role of the \(J = 2\) pairing term for the isovector MED. The TED behaviour seems far simpler and our results are consistent with the findings in \[18\] for \(\beta_r^{(2)}\) borne out in \[11\] for \(A = 46\). Therefore, here we may bet on—rather than hope for—confirmation by the charge independence breaking potentials \[13\].

The isovector channel raises a difficulty for \(A = 46\). In \[1,18\] it was found that \(\beta_r^{(1)} \approx 0\) using the same functional form as for \(\beta_r^{(2)}\) with strong \(J = 0\) pairing, which does not square with our results. But in this case our results do not square with experiment either. The scheme that has been successful in \(A = 47, 49, 50\) and \(51\) fails in \(A = 46\): we are simply unable to do any better than in \[1\] (Fig. 3a)].

The problem extends to transition rates and static moments. It was first noted and abundantly discussed in \[11\] but its quantitative explanation remains a challenge. This unsatisfactory situation provides nonetheless a helpful clue: the TED may be unsensitive to details, but the MED demand accurate wave functions and could be taken as tests of their quality.

Within the \(A = 46\) proviso, our results make obvious something that may seem at first surprising: isospin non conserving potentials play a role that is at least as important as \(V_C\) in explaining the MDE (and TDE, as found previously in \[11\]). In this respect, it is worth noting that direct evidence for charge symmetry breaking has been confined, so far, to the very little light systems (basically \(A = 2\) and \(3\)) \[8\]. The mechanism plays an important part in resolving the Nolen Schiffer anomaly in the MDE, but the effects of \(V_C\) remain much stronger \[8\]. For the MED and TED, \(V_C\) is at most as strong as \(V_f\), for which we have shown that substantial quantitative information can be extracted from the data. To boot, the MED also provide a view of the evolution of yrast radii.

This work owes much to a stay of AZ at the UAM, made possible by a scholarship of the BBVA foundation. AP is supported by grant BFM2000-30 from MCyT (Spain).

\[\begin{align*}
\text{FIG. 4: Yrast energy differences in } A = 46
\end{align*}\]