Isobaric Multiplet Yrast Energies and Isospin Nonconserving Forces

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The isovector and isotensor energy differences between yrast states of isobaric multiplets in the lower half of the *pf* region are quantitatively reproduced in a shell model context. The isospin nonconserving nuclear interactions are found to be at least as important as the Coulomb potential. Their isovector and isotensor channels are dominated by $J = 2$ and $J = 0$ pairing terms, respectively. The results are sensitive to the radii of the states, whose evolution along the yrast band can be accurately followed.

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The electrostatic energy of a sphere of radius R and charge Ze is easily calculated to be $E_C = 3e^2Z^2/5R$. It is under this guise that the Coulomb field enters the Bethe-Weizsäcker mass formula and becomes a basic quantity in nuclear structure. Direct evidence of entirely Coulomb effects has long been available from displacement energies between mirror ground states (MDE), and in the past decade from differences in *excitation* energies of yrast bands in mirror nuclei (MED) [1–6].

The MDE energies range from few to tens of MeV. They are given mainly by E_C, but precise calculations were found to be unexpectedly inaccurate—the Nolen-Schiffer anomaly [7]—and revealed the necessity to introduce charge symmetry breaking (CSB) nuclear potentials ([8] and references therein). The anomaly is now under control *to within shell effects* [9,10], which we define as deviations from a Bethe-Weiszäcker–type formula involving only number of particles (A), isospin (T), and its third component (T_z).

The MED are defined by ($Z_>$ and $Z_<$ are the largest and smallest Z in the multiplet, and E_J are the yrast excitation energies)

$$\mathrm{MED}_J = E_J(\bar{Z} + T) - E_J(\bar{Z} - T), \qquad \bar{Z} = \frac{Z_> + Z_<}{2}. \tag{1}$$

The observed MED 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 triplet energy differences (TED) given by

$$\mathrm{TED}_J = E_J(\bar{Z} + 1) + E_J(\bar{Z} - 1) - 2E_J(\bar{Z}). \tag{2}$$

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 understand this point, consider the general form of an interaction V_X defined by two body matrix elements—$V^{\pi\pi}_{Xr}$, $V^{\nu\nu}_{Xr}$, $V^{\pi\nu}_{Xr}$—written in neutron-proton ($\nu\pi$) formalism ($\boldsymbol{r} \equiv r_1 r_2 r_3 r_4$, where r_i is a subshell).

We can recast them in terms of isoscalar, $\beta^{(0)}_{Xr}$, isovector, $\beta^{(1)}_{Xr}$, and isotensor, $\beta^{(2)}_{Xr}$ contributions:

$$\beta^{(0)}_{Xr} = V^{\pi\pi}_{Xr} + V^{\nu\nu}_{Xr} + V^{\pi\nu}_{Xr}, \tag{3}$$

$$\beta^{(1)}_{Xr} = V^{\pi\pi}_{Xr} - V^{\nu\nu}_{Xr}, \qquad \beta^{(2)}_{Xr} = V^{\pi\pi}_{Xr} + V^{\nu\nu}_{Xr} - 2V^{\pi\nu}_{Xr}. \tag{4}$$

For V_C we have $\beta^{(0)}_{Cr} = \beta^{(1)}_{Cr} = \beta^{(2)}_{Cr} = V^{\pi\pi}_{Cr}$, while for V_B, $\beta^{(0)}_{Br}$ vanishes and $\beta^{(1)}_{Br}$ and $\beta^{(2)}_{Br}$ may be arbitrary.

The MED are entirely of isovector origin and the first exact shell model calculations in the full *pf* shell indicated that V^{ho}_C, 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 $V^{\mathrm{ho}}_{C\mathbf{f}_{7/2}}$ by empirical ones derived from the $A = 42$ spectrum. The ansatz (or variants of it) worked quite well, and subsequent calculations incorporated it [4,5] leading eventually to (almost) full quantitative agreement [13] for the MED in $A = 47$, 49, 50, and 51. However, it remained impossible to understand the very large differences between $V^{\mathrm{ho}}_{C\mathbf{f}_{7/2}}$ and the empirical values in terms of purely Coulomb effects. But it was equally hard to think in terms of CSB *precisely because the effects were so large*. When the isotensor TED data came in, it became clear that *both* charge independence breaking [14] and CSB had to be invoked.

Ironically, this result is obvious from the long known $A = 42$ spectra [15]. Assuming that the observed states are essentially $f^2_{7/2}$ configurations on top of the ^{40}Ca core, these spectra define an interaction in the $f_{7/2}$ subshell. The assumption of $f^2_{7/2}$ dominance is shaky, 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 $f^2_{7/2}$ centroids estimated from spectroscopic factors [15]. However, when

TABLE I. Coulomb (V_C), isovector (MED-$V_C \equiv \beta^{(1)}_{Bf_{7/2}}$), and isotensor (TED-$V_C \equiv \beta^{(2)}_{Bf_{7/2}}$) energies (keV) in $A = 42$. V_C calculated in the oscillator basis (ho).

	$J=0$	$J=2$	$J=4$	$J=6$
$V_C \equiv V^{\rm ho}_{Cf_{7/2}}$	81.60	24.60	6.40	−11.40
$E_J[^{42}\mathrm{Ti} - {}^{42}\mathrm{Ca}] - V_C$	5.38	92.55	4.57	−47.95
$E_J[^{42}\mathrm{Ti} + {}^{42}\mathrm{Ca} - 2\,{}^{42}\mathrm{Sc}] - V_C$	116.76	80.76	2.83	−42.15

this is done, no significant change is obtained, and the numbers we analyze correspond to the yrast energies.

The first line of Table I shows the matrix elements $V^{\rm ho}_{Cf_{7/2}}$, which will be taken to be a fair representation of V_C [16]. Since MED(observed) $= \beta^{(1)}_{Cf_{7/2}} + \beta^{(1)}_{Bf_{7/2}}$, by subtracting $V_C \approx \beta^{(1)}_{Cf_{7/2}}$ we obtain in the second line of Table I an estimate of $\beta^{(1)}_{Bf_{7/2}}$. Similarly, the third line gives $\beta^{(2)}_{Bf_{7/2}}$. The inevitable conclusion is that *the role of isospin nonconserving 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 [17] 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 [18]). The energy differences are obtained in first order perturbation theory [19], as sums of expectation values, in which we separate the monopole and multipole components of the Coulomb field $V_C = V_{Cm} + V_{CM}$ following Refs. [10,13]:

$$\mathrm{MED}_J = \Delta_{\rm M}\langle V_{Cm}\rangle_J + \Delta_{\rm M}\langle V_{CM}\rangle_J + \Delta_{\rm M}\langle V_B\rangle_J, \qquad (5)$$

$$\mathrm{TED}_J = \Delta_{\rm T}\langle V_{CM}\rangle_J + \Delta_{\rm T}\langle V_B\rangle_J. \qquad (6)$$

The monopole V_{Cm} contains all terms quadratic in scalar products of fermion operators $a^+_i \cdot a_j$. In [10] it is shown that the diagonal contributions ($i = j$) amount to essentially E_C plus a single particle splitting induced by V_C on the orbits of principal quantum number p above harmonic oscillator closed shell $Z_{\rm cs}$ [10]:

$$\varepsilon_{Cl} = \frac{-4.5 Z_{\rm cs}^{13/12}[2l(l+1) - p(p+3)]}{A^{1/3}(p+3/2)}\ \text{keV}. \qquad (7)$$

We shall ignore the nondiagonal contributions ($i \neq j$) that lead to higher order corrections and isospin mixing.

The effect of E_C is proportional to the difference of (inverse) radii between a J yrast and the ground state [5]. 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 $\langle m_k\rangle_J/2$, 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 [10]. As it is reasonable (and consistent with experiment [15]) 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 ε_{Cl} from Eq. (7) is proportional to the *difference of proton and neutron* occupancies. It is typically 10 times smaller than the radial effect in $A = 47$–51, so we neglect it and end up with $\Delta_M\langle V_{Cm}\rangle_J = a_m\langle m_{p_{3/2}}\rangle_J/2$. However, in $A = 41$ the contribution of ε_{Cl} is significant and makes it possible to estimate a_m. From (7) we find that the $l = 3$ orbits are depressed with respect to the $l = 1$ ones by 150 keV at $A = 41$, $Z_{\rm cs} = 20$. The radial effect acts in the opposite direction: for small l, the radii are larger and the E_C repulsion weaker. As the observed splitting is 200 keV, we end up with $a_m \approx 200 + 150 = 350$ keV.

The isotensor $m_{p_{3/2}}$ contributions cancel out.

The multipole contribution $\Delta\langle V_{CM}\rangle_J$ is calculated using oscillator Coulomb matrix elements in the pf shell [20].

The only direct information on V_B comes from Table I. To make use of it, we must explore the possibility of specifying an interaction acting in the full pf shell, *solely in terms of $f_{7/2}$ matrix elements*. In some cases, the idea turns out to be quite viable using a multiplicative prescription [21]

$$\Delta\langle V_{X\mathbf{pf}}\rangle_J = b\Delta\langle V_{X\mathbf{f}_{7/2}}\rangle_J, \qquad (8)$$

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 $V^{J=0 \text{ or } J=2}_{\mathbf{f}_{7/2}}$ matrix elements. Since these are the leading terms suggested by Table I, we have taken the blunt step of retaining only them in our definition of V_B, setting $\beta^{(1)}_{B\mathbf{pf}} = \beta_1 V^{J=2}_{\mathbf{f}_{7/2}}$, $\beta^{(2)}_{B\mathbf{pf}} = \beta_2 V^{J=0}_{\mathbf{f}_{7/2}}$, where $V^J_{\mathbf{f}_{7/2}}$ is the matrix element with unit value. Collecting all the pieces, we have

$$\mathrm{MED}_J = \tfrac{1}{2}a_m\langle m_{p_{3/2}}\rangle_J + \Delta_{\rm M}\langle V^{\rm ho}_{C\mathbf{pf}} + \beta_1 V^{J=2}_{\mathbf{f}_{7/2}}\rangle_J, \qquad (9)$$

$$\mathrm{TED}_J = \Delta_{\rm T}\langle V^{\rm ho}_{C\mathbf{pf}} + \beta_2 V^{J=0}_{\mathbf{f}_{7/2}}\rangle_J. \qquad (10)$$

In Figs. 2 for the MED, V_{Cm}, V_{CM}, and V_{BM} stand,

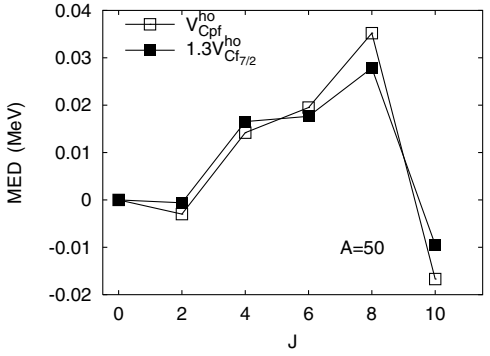

FIG. 1. The two terms of Eq. (8) for V_C in $A = 50$.

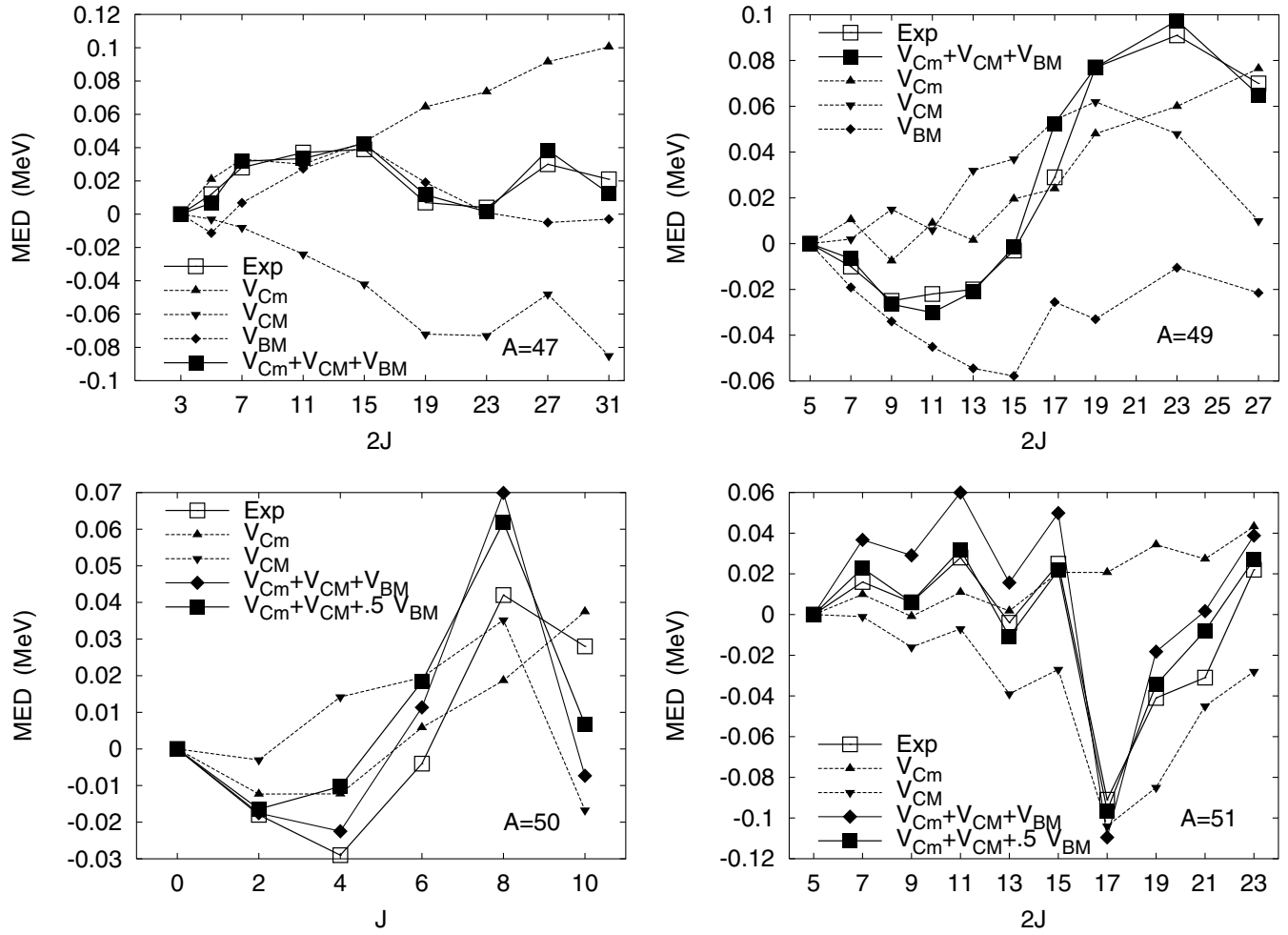

FIG. 2. Experimental [2–5] and calculated MED for the pairs ^{47}V-^{47}Cr, ^{49}Cr-^{49}Mn, ^{50}Cr-^{50}Fe, and ^{51}Mn-^{51}Fe.

respectively, for the first, second, and third terms in Eq. (9). We have chosen round numbers, $a_m = 300$ keV, consistent with the 350 keV estimate, and $\beta_1 = \beta_2 = 100$ keV, consistent with the matrix elements in Table I. The enormous advantage of these prescriptions is that the calculations become parameter free.

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. (8) and Fig. 1—we expect a case by case (even matrix element by 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.

The V_{Cm}, V_{CM}, and V_{BM} contributions, shown separately in Fig. 2 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 in the plots the V_{BM} part by the full contribution with β_1 halved. For $A = 50$ the changes are insignificant, but there is a definite improvement in $A = 51$ [remember again Eq. (8) and Ref. [25]].

It is especially worth noting in Fig. 2 that the strong signature effect in the $A = 49$ band is erased in the MED by the out-of-phase V_{Cm} and V_{CM}, while the signature staggering is enhanced in $A = 51$.

The experimental TED patterns in Fig. 3 are quite nicely reproduced by the minimal $\beta^{(2)}_{B\mathbf{pf}} = \beta_2 V^{J=0}_{\mathbf{f}_{7/2}}$ choice. As mentioned, the inclusion of the $J \neq 0$ terms (third line

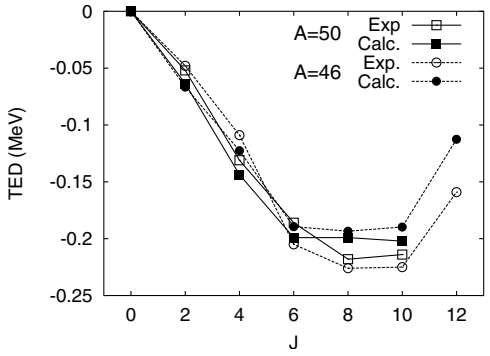

FIG. 3. TED for $A = 46$ and 50.

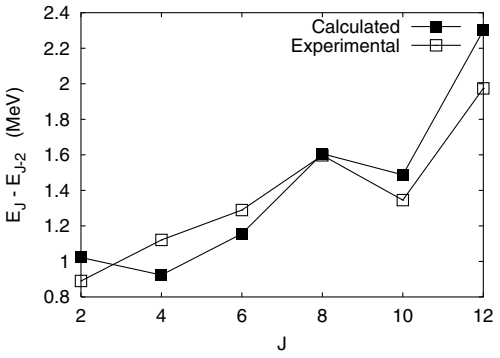

FIG. 4. Yrast energy differences in $A = 46$.

of Table I) makes little difference, and—interestingly enough—simply *ignoring* V_B and *doubling* V_{CM} (or the other way around) makes practically no difference, which confirms the overwhelming dominance of $J = 0$ pairing.

It can be hoped that a rigorous treatment calling upon state of the art CSB potentials [8] will confirm the role of the $J = 2$ pairing term for the isovector MED. The TED behavior seems far simpler and our results are consistent with the findings in [23] for $\beta^{(2)}_{B\mathbf{pf}}$ borne out in [12] for $A = 46$. Therefore, here we may bet on—rather than hope for—confirmation by the charge independence breaking potentials [14].

The isovector channel raises a difficulty for $A = 46$. In [12,23] it was found that $\beta^{(1)}_{B\mathbf{pf}} \approx 0$ using the same functional form as for $\beta^{(2)}_{B\mathbf{pf}}$ 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 Fig. 3a of [12].

The trouble is no doubt due to the poor spectroscopy provided by full pf shell diagonalizations for $A \leq 46$, at least when compared with the very high quality descriptions for the rest of the $f_{7/2}$ nuclei (i.e., $A \leq 56$). Figure 4 illustrates the point: the calculated yrast energetics is wrong for the lowest states and, for the others, far less precise than the corresponding patterns in the heavier nuclei (see, for example, [24] for $A = 47$ and 49). This problem extends to transition rates and static moments. It was first noted and abundantly discussed in Ref. [25] but its quantitative explanation remains a challenge. This unsatisfactory situation provides nonetheless a helpful clue: the TED may be insensitive 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 nonconserving potentials play a role that is at least as important as V_C in explaining the MDE (and TDE, as found previously in [12]). In this respect, it is worth noting that *direct* evidence for charge symmetry breaking has been confined, so far, to the *very* 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 [10]. For the MED and TED, V_C is at most as strong as V_B, for which we have shown that substantial quantitative information can be extracted from the data. In addition, the MED also provide a view of the evolution of yrast radii.

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