Isobaric analog state in the f_{7/2} and g_{9/2} shells

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Calculations are performed for energies of isobaric analog states with isospins T=2 and T=3 in regions where they have been found experimentally e.g. f-p shell, and regions where they have not yet been found e.g. g_{9/2} near Z=50,N=50. We consider two approaches—one using binding energy formulas and Coulomb energies contained therein and the other using shell model calculations. It is noted that some (but not all) calculations yield very low excitation energies for the J=0^+T=2 isobaric analog state in ^{96}Ag.

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If there were no violation of charge independence, the binding energy of the ^{96}Pd ground state (J = 0^+, T = 2) would be identical to the binding energy of the analog state, also J = 0^+, T = 2, in ^{96}Ag. But, since that is not the case in real life, the excitation energy of the J = 0^+, T = 2 state in ^{96}Ag is given by

\[ E^*(J = 0^+, T = 2) = BE(^{96}Ag) - BE(^{96}Pd) + V_C, \]

where the BEs are the binding energies and V_C includes all charge-independence violating effects. The binding energies can be obtained from the latest mass evaluation [1] and we assume that V_C arises from the Coulomb interaction, which must be estimated.

We use the classical form of the Coulomb energy

\[ E_C = \alpha_C Z^2/A^{1/3}, \]

supplemented by an exchange Coulomb term

\[ E_{xc} = \alpha_{xc} Z^4/A^{1/3}, \]

where \( \alpha_C \) and \( \alpha_{xc} \) are coefficients to be obtained from appropriate data. Several sources were compared. The simplest is the Bethe-Weizsäcker semi-empirical mass formula [2, 3], which produces \( \alpha_C = 0.691 \) MeV, \( \alpha_{xc} = 0 \) from a fit of a four-term semi-empirical mass formula to the measured masses. An extended, ten-term mass formula [3] produces \( \alpha_C = 0.774 \) MeV and \( \alpha_{xc} = -2.22 \) MeV from a similar fit. The best mass formulation currently available is the Duflo-Zuker approach [1, 3] with up to 33 parameters fitted to the mass data. It includes a unified Coulomb term

\[ E_C^{\text{DZ}} = \alpha_C \frac{Z(Z-1) - 0.76[Z(Z-1)]^{2/3}}{A^{1/3}} \left[ 1 - \frac{(N-Z)^2}{4A^{2/3}} \right] \]

and the best fits to the data have \( \alpha_C = 0.700 \) MeV.

Binding energy differences of mirror nuclei, together with Coulomb displacement energies, can be fitted to differences of \( E_C \) and \( E_{xc} \) (eqs. (2), (3)), from which \( \alpha_C = 0.717 \) MeV and \( \alpha_{xc} = -0.928 \) MeV [3]. The formula of Anderson et al. [6]:

\[ V_C = E_1 \overline{Z}/A^{1/3} + E_2, \]

where \( \overline{Z} = (Z_1 + Z_2)/2 \), is a semi-empirical representation of the same data, as far as it was known at the time. Anderson et al. [6] list several sets of values of \( E_1 \) and \( E_2 \). We here use the average values \( E_1 = 1.441 \) MeV and \( E_2 = -1.06 \) MeV.

Table IV compares the Coulomb energy estimates, using the different prescriptions presented above, for a number of nuclei of interest for this discussion of analog state excitation energy. Though estimates of the total Coulomb energy can vary strongly between prescriptions, the differences which are relevant to the analog states show much less variability. In particular, estimates which are based on fits to mirror nuclei and Coulomb displacement energies agree very closely among themselves. The Anderson et al fit has stood the test of time remarkably well.

With relatively stable Coulomb energy differences in hand and with experimental binding energies, we are able to compute, using eq. (4), predicted excitation energies of analog states, and can compare the results with measured
Table I: Coulomb energy estimates for some nuclei, in MeV. Lines labeled $A = \ldots$ give the differences of the two preceding lines.

| Nucleus | Bethe-Weizsäcker | Ten-term | Duflo-Zuker | Mirror/CDE | Anderson et al |
|---------|------------------|----------|-------------|------------|---------------|
| $^{44}$Sc | 86.318           | 60.253   | 74.872      | 74.336     |                |
| $^{44}$Ca | 78.293           | 53.558   | 67.586      | 66.968     |                |
| $A = 44$ | 8.052            | 6.694    | 7.285       | 7.368      | 7.308          |
| $^{46}$Sc | 85.048           | 59.366   | 73.872      | 73.242     |                |
| $^{46}$Ca | 77.141           | 52.771   | 66.738      | 65.983     |                |
| $A = 46$ | 7.907            | 6.596    | 7.134       | 7.259      | 7.185          |
| $^{52}$Mn | 115.706          | 86.126   | 102.432     | 101.885    |                |
| $^{52}$Cr | 106.635          | 78.268   | 94.079      | 93.435     |                |
| $A = 52$ | 9.071            | 7.858    | 8.353       | 8.450      | 8.399          |
| $^{60}$Cu | 148.442          | 115.748  | 133.491     | 132.907    |                |
| $^{60}$Ni | 138.381          | 106.788  | 124.048     | 123.433    |                |
| $A = 60$ | 10.061           | 8.960    | 9.362       | 9.474      | 9.430          |
| $^{94}$Rh | 307.747          | 266.563  | 286.532     | 286.658    |                |
| $^{94}$Ru | 294.221          | 253.719  | 273.683     | 273.588    |                |
| $A = 94$ | 13.526           | 12.843   | 12.849      | 13.070     | 13.043         |
| $^{96}$Ag | 333.362          | 291.169  | 311.153     | 311.530    |                |
| $^{96}$Pd | 319.328          | 277.773  | 297.738     | 297.939    |                |
| $A = 96$ | 14.035           | 13.396   | 13.415      | 13.591     | 13.574         |

Table II: Excitation energies of isobaric analog states in MeV.

| NUCLEUS | Binding Energy Difference | Coulomb Energy | Excitation Energy | Single $j$ | Large space | Experiment |
|---------|---------------------------|----------------|-------------------|------------|-------------|------------|
| $^{44}$Sc | 4.435                     | 7.308          | 2.873             | 3.047$^a$  | 3.418$^b$   | 2.779      |
| $^{46}$Sc | 2.160                     | 7.185          | 5.024             | 4.949$^a$  | 5.250$^b$   | 5.022      |
| $^{52}$Mn | 5.494                     | 8.399          | 2.905             | 2.774      | 2.7307      | 2.926      |
| $^{60}$Cu | 6.910                     | 9.430          | 2.520             | 2.235      | 2.726$^b$   | 2.536      |
| $^{94}$Rh | 10.458                    | 13.043         | 2.585             | 1.990$^c$  | 3.266$^d$   |            |
| $^{96}$Ag | 12.453                    | 13.574         | 1.121             | 0.900$^c$  | 1.9167$^d$  |            |

$^a$Escuderos, Zamick, Bayman (2005) [7].
$^b$GXPF1 interaction [8].
$^c$Zamick and Escuderos (2012) [9].
$^d$ji4b interaction [10].
$^e$CCGI interaction [9, 11].
$^f$JUN45 interaction [12].
$^g$truncated model space, allowing 4 nucleons excited from the $f_{7/2}$ subshell

Excitation energies, where they exist. We show in Table II results for various nuclei, some for which the excitation energy of the analog state is known and some for which it is not. The binding energy differences $\text{BE}(Z,N)-\text{BE}(Z+1,N-1)$ are taken from Ref. 1, the Coulomb energy differences from the Anderson et al semi-empirical fit [6].

In all four cases where the excitation energy of the analog state is known, our prediction agrees with the experimental value within 100 keV, and for three of them, within 25 keV. The fact that the analog state and Coulomb arguments work well in known cases gives us confidence that we can use these for the unknown case of $^{96}$Ag, where we predict an excitation energy just slightly above 1 MeV. Turning things around, if the isobaric analog state were found, then we might have a better constraint on what the binding energy is.

We can compare our predicted excitation energies with selected calculations in the literature (included in Table II). We look at shell-model calculations of two basic kinds — single-$j$ or large-space — and with various effective interactions. For $^{44}$Sc and $^{46}$Sc, single-$j$-shell results ($f_{7/2}$) [7] are respectively 3.047 and 4.949 MeV, as compared with Table II's excitation energies of 2.873 and 5.024 MeV. The large space results are also shown. In $^{52}$Mn there is
Table III: Excitation energies of isobaric analog states (in MeV) based on mass formulas, for comparison with predicted analog state energy in Table II.

| NUCLEUS | 5-term Binding Energy | 5-term Analog Energy | 10-term Binding Energy | 10-term Analog Energy | Duflo-Zuker Binding Energy | Duflo-Zuker Analog Energy |
|---------|-----------------------|----------------------|-----------------------|-----------------------|--------------------------|--------------------------|
| 44Sc    | 5.499                 | 2.526                | 4.768                 | 1.926                 | 4.934                    | 2.351                    |
| 46Sc    | 1.650                 | 6.257                | 2.035                 | 4.624                 | 2.440                    | 4.694                    |
| 52Mn    | 7.200                 | 1.871                | 6.460                 | 1.398                 | 6.472                    | 1.881                    |
| 60Cu    | 8.653                 | 1.408                | 7.968                 | 0.992                 | 7.015                    | 2.347                    |
| 94Rh    | 11.208                | 2.318                | 11.361                | 1.482                 | 10.837                   | 2.012                    |
| 96Ag    | 13.668                | 0.367                | 13.453                | -0.057                | 12.885                   | 0.530                    |

reasonable agreement between predicted, single-j, large space and experiment. In the small space for \(^{60}\)Cu \((p_{3/2})\) we can use a particle-hole transformation to get the spectrum of this nucleus from the spectrum of \(^{58}\)Cu since three \(p_{3/2}\) neutrons can be regarded as a single neutron hole. This gives a value of 2.235 MeV as compared with the experimental value of 2.356 MeV.

For \(^{96}\)Ag single-j-shell results \[9\] are 0.900 MeV with \(\text{INTd}\) and 0.842 MeV with the \(\text{CCGI}\) interaction \[9, 11\]. These are lower than the excitation energy in Table II of 1.121 MeV. There are also large scale calculations with the \(\text{j}\)\(\text{j}\)\(\text{4}\)\(\text{4}\)\(\text{b}\) interaction for \(^{96}\)Ag—the result is 1.917 MeV, significantly larger than the predicted value. In \(^{94}\)Rh the \(\text{j}\)\(\text{j}\)\(\text{4}\)\(\text{4}\)\(\text{b}\) interaction yields 3.266 MeV, larger than Table II's predicted value of 2.585 MeV. The large space calculations with \(\text{JUN45}\) are qualitatively similar. The single-j \(\text{INTd}\) and \(\text{CCGI}\) results are lower, 1.990 MeV and 2.048 MeV respectively.

Although it is clearly preferable to base predictions of the excitation energy of the analog state on experimentally measured binding energies, it may become necessary to use binding energies derived from mass formulas where data is unavailable. To this end, we check how susceptible these predictions are to various mass formulas. We tested the mass formulas used above to obtain Coulomb energy differences — a 5-term Bethe-Weizsäcker formula (the standard four terms, supplemented with a pairing term), its 10-term extension, and the 33-parameter Duflo–Zuker mass formulation.

The results for the analog states are presented in Table III. In all cases, the Coulomb energy differences were obtained from the respective binding energy formulas.

The Duflo-Zuker results are closest to the predictions based on the atomic mass evaluation (fourth column of Table II). As might have been expected, mass formulas with smaller rms deviations from the measured data are better predictors of the analog state excitation energy. Even so the calculated value for \(^{52}\)Mn (1.881 MeV) is considerably lower than the experimental value (2.926 MeV).

Why study isobaric analog states? One reason has to do with the strange dualism in nuclear structure that has emerged over the years. For the most part calculations of the excited states of nuclei have been performed with little mind to the binding energies or saturation properties. On the other hand binding energies and nuclear densities are addressed in Hartree-Fock calculations with interactions for which it makes no sense to calculate nuclear spectra. With isobaric analog state energies we have an in your face confrontation of these two approaches. As shown in Eq. (1) one needs good binding energies and good Coulomb energies to correctly predict the excitation energies of these states. As has been noted in ref \[9\] with the shell model one can get very impressive fits for many energy levels in say \(^{96}\)Ag but no one has even tried to calculate the energy of the isobaric analog state here until now. Hopefully our work will stimulate trying to get a unified approach in which both the spectra and bulk properties of nuclei are treated in a unified manner.

Another point of interest is the possibility that in some region of the periodic table the \(T=2\) isobaric analog state would become the ground state. In Table III the 10 point formula yields such a result. If this were indeed the case there would be a drastic difference in the decay mode of the nucleus in question. Instead of the usual decay mode — electron capture — one would now have an allowed Fermi transition. This would lead to a much shorter lifetime and could influence how the elements evolve. This does not occur in \(^{96}\)Ag where it is known that the decay mode is electron capture but it might occur in heavier nuclei. For example \(Z=66, A=132\) closes the \(\text{h}_{11/2}\) shell. Consider a very proton rich nucleus with \(A=128\) and \(Z=63\), a nucleus with 3proton holes and one neutron hole. The excitation energies for 5- term, 10-term and Duflo-Zuker are respectively -0.009, 1.251 and 0.366 MeV.

Before leaving we would briefly like to defend out inclusion of small space calculations in Table II. There is a precedent for this in the work of Talmi and collaborators \[14\]. They obtain excellent agreement with binding energies in several regions, e.g. the \(\text{Ca}\) isotopes, using a single j-shell formula but with phenomenological parameters. We here adopt the same philosophy of obtaining two body matrix elements from experiment. Matrix elements form experiment implicitly contain not all but many nuclear correlations.

In view of the differing results of shell model calculations and mass formulas it would be of great interest to
measure the excitation energies of isobaric analog states in the $g_{9/2}$ region. We hope that this work will encourage experimentalists to look not only for the surprisingly neglected $J = 0^+$ isobaric analog states in $^{94}$Rh and $^{96}$Ag, but also for other such states throughout this region.

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