Isospin nonconservation for fp-shell nuclei by spectral distribution theory

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ABSTRACT

The one- plus two-body isospin nonconserving nuclear interactions are included in the prediction of ground state energies of fp shell nuclei using spectral distribution theory. This in turn is used to calculate the linear term in the isobaric mass-multiplet equation and the predictions are then compared to experimental values after the addition of the Coulomb contribution. The agreement is found to be reasonable as observed for sd shell nuclei earlier. One also sees that in this method the contribution to the linear term comes almost completely from the one body isovector Hamiltonian and that results in a huge simplification of the problem.

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Though isospin symmetry is one of the most well-known symmetries in nuclear structure and using the goodness of isospin quantum number considerable simplifications are obtained in nuclear structure calculations, the small breaking of this symmetry by nuclear interactions has been observed and experimentally measured over the years. Wigner [1] was the first one to postulate an isobaric mass multiplet equation (IMME) which quantitatively describes the isospin non-conservation and is given by

\[
M(\alpha, T, T_z) = a(\alpha, T) + b(\alpha, T)T_z + c(\alpha, T)T_z^2
\]  

(1)

where \( M(\alpha, T, T_z) \) stands for the masses of the nuclei in a multiplet with fixed isospin \( T \) and \( T_z = (N - Z)/2 \) takes values \( -T, -T+1, \ldots, T-1, T \). Thus the equation stands for the masses of \( (2T+1) \) isobars. The parameters ‘a’, ‘b’ and ‘c’ are often evaluated by fits to experimental values. For microscopic nuclear structure calculations like the shell model one writes the total Hamiltonian \( (H) \) as not only the symmetry-preserving isoscalar one- and two-body parts \( (H^{(0)}) \) but with the addition of the one- and two-body isovector \( (H^{(1)}) \) and the two-body isotensor \( (H^{(2)}) \) parts. Many shell model and other calculations have been carried out for light nuclei in the \( p \)-shell, \( sd \)-shell, \( fp \)-shell \[2\] \[3\] and the theoretical predictions for ‘b’ and ‘c’ of IMME compared to the experimental numbers. Ormand and Brown have pointed out that the parameter ‘b’ times ‘\( T_z \)’ is exactly equal to the contribution to the ground state coming from the isovector Hamiltonian \[2\].

Spectral distribution theory \[4\] \[5\] \[6\] \[7\] \[8\] \[9\] \[10\] \[11\] describes the statistically averaged nuclear structural properties avoiding explicit diagonalisation of the Hamiltonian and calculates the relevant quantities evaluating traces of operators and product of operators in the shell model spaces. It has been applied successfully to calculate spectra and energy-averaged transition strengths of light nuclei \[11\] \[12\]. This theory has recently been extended to include non-isoscalar one- and two-body interactions and a methodology developed to calculate the linear term in the IMME \[13\]. Examples of nuclei in the \( sd \)-shell show that the theory works quite well in predicting the parameter ‘b’ in IMME. In this work we consider nuclei belonging to the \( fp \)-shell and observe that the theory is reasonably successful for these nuclei as well. We also see that using the Ormand-Brown interaction and their parametrisation \[2\] the prediction for the linear term changes very little when one neglects the two body parts in the isovector and isotensor Hamiltonians. This was observed earlier for \( sd \)-shell nuclei too \[13\].

In spectral distribution theory one observes that with ‘\( m \)’ valence particles coupling to total isospin ‘\( T \)’, the eigenvalue density of all realistic Hamiltonians in the configuration shell model spaces is very close to Gaussian as long as the dimension of each of this space is large. So the energy intensities \( I_{m,T}(E) \), defined as the energy eigenvalue density \( \rho_{m,T} \) times the dimension of the configuration space \( d(m, T) \) adding up to give the total intensity \( I_{m,T}(E) \), are functions of only two quantities, the centroid and the width for each configuration. So the total intensity is given by

\[
I_{m,T}(E) = \sum_m I_{m,T}(E) = \sum_m d(m, T)\rho_{m,T}(E)
\]  

(2)

Once one is able to calculate the fixed T configuration centroids and widths in this theory by using the unitary group structure of the shell model spaces with ‘\( m \)’ particles distributed over ‘\( l \)’
valence orbits (for the \(fp\)-shell case the orbits are \(0f_{5/2}, 0f_{7/2}, 1p_{3/2}\) and \(1p_{1/2}\)) one knows the eigenvalue densities and the intensities.

Though the spectral distribution theory describes the global averaged properties, it can give information of the microscopic states like the ground state and the low-lying spectra. The ground state energy of a nucleus with a fixed number of valence particles and isospin is evaluated by a method named the Ratcliff procedure \[14\]. If \(d_i\) is the degeneracy of the \((i-1)\)-th excited state (\(d_1\) being the degeneracy of the ground state) the energy of that state \(\bar{E}_i\) is obtained by inverting the equation

\[
\sum_m \int_{-\infty}^{E_i} I_{m,T}(E)dE = \sum_{k=1}^{i-1} d_k + d_i/2
\]  

The calculated energy of the ground state \(\bar{E}_1\) will be denoted by the more familiar symbol \(E_g\). We calculate the ground state energies by spectral distributions for the cases \((m = 3, T = 1/2), (m = 5, T = 1/2)\) and \((m = 6, T = 1)\) with \(^{40}\text{Ca}\) as the closed core, using the \(fp\)-shell FPV interaction \[15\]. These calculations are constrained to have only one particle outside the \(0f_{7/2}\) orbit following Table 1 of Ref. \[2\] and so we choose only such configurations for our calculations for all the three cases. We first convert the two-body matrix elements from the \((JT)\) form in the 4 orbits to the proton-neutron form in 8 orbits (4 proton orbits plus 4 neutron orbits). The expressions for the pp, nm and pn/np matrix elements for the isoscalar interactions are wellknown \[16\] and those for the isovector and isotensor interaction are given by Ormand and Brown \[2\] and discussed by Kar and Sarkar \[13\]. The centroids and widths in the configurations are obtained by evaluating traces using the group theoretical structure of the configuration-pn spaces first \[11\] and then in configurations with fixed isospin by the method of subtraction of the traces \[16\] \[17\] \[13\].

Table 1 gives the centroids and widths in all the 4 fixed isospin configurations considered with the FPV interaction for the isoscalar Hamiltonian and compares them with the values for the total Hamiltonian. We observe, that in all the cases, with the addition of the isovector and isotensor parts, the centroids move away from the values with only isoscalar but the widths remain almost the same.

In Table 2 we present the ground state energies of the 3, 5 and 6 particle cases calculated by the method described above. Values are given for both the isoscalar \(H\) and the total \(H\) in fixed isospin spaces as well as for spaces with fixed proton and neutron numbers (taking \(T_z = T\)). The coefficient \(b\) in the linear term in the IMME is obtained by equating the difference between the calculated lowest \((m, T, J)\) state energy with the isoscalar plus isovector Hamiltonian \(H^{(0)\ast} + H^{(1)}\) and only the isoscalar Hamiltonian \(H^{(0)}\) to \(bT_z\). The contribution of the Coulomb term to \(b\) can be evaluated by using the equation (25) of Lam, Smirnova and Caurier \[3\]. However in this work we use for \(b\) coming from Coulomb energy, the expression given by the equation (10) in the work of Ormand \[18\] which is a global fit with good accuracy. The experimental values are as quoted in Ormand and Brown \[2\]. For the 5 particle case alongwith the \(J = 7/2\) ground state the table also presents the values for the first and second excited states with \(J = 3/2\) and \(J = 5/2\) respectively. We find the agreement of our results with experimental values reasonable keeping in mind that spectral distribution theory is constructed to describe the statistically averaged global properties of nuclei.
| Fixed T configuration | Dimension | Isoscalar H centroid (MeV) | Isoscalar H width (MeV) | Total H centroid (MeV) | Total H width (MeV) |
|-----------------------|-----------|---------------------------|------------------------|-----------------------|-------------------|
| (1200)                | 384       | -21.12                    | 2.16                   | -24.83                | 2.16              |
| (0300)                | 168       | -27.39                    | 2.07                   | -31.10                | 2.07              |
| (0210)                | 256       | -25.34                    | 1.85                   | -29.00                | 1.85              |
| (0201)                | 128       | -23.55                    | 1.88                   | -27.22                | 1.88              |
| (1400)                | 4284      | -42.42                    | 3.37                   | -46.13                | 3.37              |
| (0500)                | 1080      | -48.46                    | 3.27                   | -52.17                | 3.27              |
| (0410)                | 2856      | -46.05                    | 3.13                   | -49.73                | 3.13              |
| (0401)                | 1428      | -44.37                    | 3.15                   | -48.05                | 3.15              |
| (1500)                | 9072      | -52.81                    | 3.71                   | -60.22                | 3.71              |
| (0600)                | 1512      | -59.11                    | 3.49                   | -66.52                | 3.49              |
| (0510)                | 6048      | -56.34                    | 3.48                   | -63.70                | 3.48              |
| (0501)                | 3024      | -54.69                    | 3.50                   | -62.05                | 3.50              |

Table 1: Centroids and widths of the isoscalar Hamiltonian compared to the centroids and widths of the total Hamiltonian (including the isovector and istensor parts) in the fixed-T configurations with 3, 5 and 6 particles in 0f – 1p shell with $T = 1/2$, $T = 1/2$ and $T = 1$ respectively. The notation $(m_1, m_2, m_3, m_4)$ stands for the configuration with $m_1$ particles in orbit $0f_{5/2}$, $m_2$ particles in orbit $0f_{7/2}$, $m_3$ particles in orbit $1p_{3/2}$ and $m_4$ in orbit $1p_{1/2}$.

| $(m,T,J)$ | LSE for $H^{(0)}$ (MeV) | LSE for Total H $(H^{(0)} + H^{(1)})$ (MeV) | $b$ from Total H (MeV) | $b$ for Coulomb (MeV) | Total $|b|$ (MeV) | Observed $|b|$ (MeV) |
|-----------|-------------------------|-----------------------------------------------|------------------------|-----------------------|-----------------|-----------------|
| (3,1/2,7/2) | -31.52 (-31.30) | -35.21 (-35.00) | -35.21 | -7.38 | -0.41 | 7.79 | 7.650 |
| (5,1/2,7/2) | -57.30 (-56.97) | -61.01 (-60.68) | -61.00 | -7.40 | -0.68 | 8.08 | 7.914 |
| (5,1/2,3/2)* | -56.56 (-56.28) | -60.26 (-59.98) | -60.26 | -7.40 | -0.68 | 8.08 | 7.934 |
| (5,1/2,5/2)* | -55.92 (-55.69) | -59.63 (-59.39) | -59.62 | -7.40 | -0.68 | 8.08 | 7.930 |
| (6,1,0) | -71.16 (-70.90) | -78.57 (-78.31) | -78.57 | -7.41 | -0.81 | 8.22 | 8.109 |

Table 2: The parameter ‘$b$’ of IMME coming from nuclear interactions from evaluation of the lowest state energies (LSE) calculated by spectral distributions. The Coulomb contribution is calculated using eq (25) of ref [3]. The numbers in the parentheses are LSEs calculated in the $(m_p, m_n)$ spaces. The states with the (*) are not the ground states but the lowest $(m = 5, T = 1/2)$ states with $J = 3/2$ and $J = 5/2$ whereas the other 3 are ground states.

| A | T | $|b|$ by Spectral Distributions | $|b|$ by Spectral Distributions with Isoscalar and 1-body Isovector | Observed $|b|$ |
|---|---|-------------------------------|---------------------------------------------------------------|-------------|
| 43 | 1/2 | 7.79 | 7.79 | 7.65 |
| 45 | 1/2 | 8.08 | 8.09 | 7.91 |
| 46 | 1 | 8.22 | 8.23 | 8.11 |

Table 3: Comparison of $|b|$ using isoscalar with only one-body isovector Hamiltonian with $|b|$ from the full H.
Finally in Table 3, we show the results for ‘b’ when we include only the one-body isovector $H^{(1)}$ and not the two-body part in our calculations. We compare them with the results given in Table 2 where both the one- and two-body parts of $H^{(1)}$ are included. One observes that there is hardly any change in the results when one drops the two-body isovector part. This feature was observed for the $sd$-shell nuclei in the earlier work of Kar and Sarkar [13]. This originates from the fact the overall multiplicative coefficient in the two-body isovector Hamiltonian of Ormand and Brown [2] which is used by us, is very small. But this parametrisation of the Hamiltonian had resulted in shell model predictions which were very accurate [2]. The fact that the two body part need not be included for calculating the linear term of IMME is an enormous simplification and may be followed up for other nuclei in future.

In conclusion, we observe that the linear term in the isobaric mass-multiplet equation for isospin-breaking can be calculated by the spectral distribution theory and its predictions agree well with the available data for the $fp$-shell nuclei as well, seen earlier to work well for the $sd$-shell nuclei.

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