Pramana – J. Phys. (2020) 94:100
https://doi.org/10.1007/s12043-020-01957-2

The linear term in the isobaric-mass-multiplet equation for *fp*-shell nuclei in the framework of spectral distribution theory

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MS received 15 March 2018; revised 26 May 2019; accepted 13 March 2020

Abstract. The one- plus two-body isospin non-conserving nuclear interactions, namely the isovector and isotensor ones, are included in the prediction of the energies of the ground state and the low-lying states of the *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 with experimental values after the addition of the Coulomb contribution. The agreement is found to be good 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, resulting in a huge simplification of the problem.

Keywords. Isospin non-conservation; *fp* shell; spectral distribution theory.

PACS Nos 21.10.Hw; 21.30.−x; 21.60.−n; 21.60.Fw

1. Introduction

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. A small breaking of this symmetry by nucleon–nucleon interactions has been observed and experimentally measured over the years. This breaking of course comes from the electromagnetic Coulomb interaction, but the isovector and the isotensor nuclear interactions also contribute to this breaking. The isovector interaction can connect a given state (with isospin T) to states with isospin differing by one from the original state ($T' = T \pm 1$). The isotensor interaction has non-zero matrix elements between states differing in isospin values up to two, i.e. $\left|T' - T\right| \leq 2$. 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

$$M(\alpha, T, T_z) = a(\alpha, T) + b(\alpha, T)T_z + c(\alpha, T)T_z^2, \quad (1)$$

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 can write 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 with isoscalar interactions in p-shell, sd-shell, fp-shell [2,3] and then the change in energy eigenvalue due to the isovector and isotensor nuclear interactions evaluated by first-order perturbation theory [2]. The theoretical predictions for b and c of IMME thus obtained are then compared with 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 [4–11] 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

Published online: 09 July 2020

nuclei [11,12]. This theory has recently been extended to include non-isoscalar one- and two-body interactions and a methodology was developed to calculate the linear term in IMME [13]. The linear term is obtained from the change in energy of the low-lying states due to the isovector and the isotensor terms, but the spectral distribution cannot calculate wave functions and the isospin mixing in them. 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 successful for these nuclei as well. We find that using the interaction and the parametrisation as used by Ormand and Brown [2], the contributions of the two-body parts are more than an order of magnitude smaller than the ones from one-body term and the predictions for the linear term in IMME changes very little when one neglects the two-body parts in the isovector and isotensor Hamiltonians. Thus, without losing much accuracy, b can be evaluated by taking only a one-body isovector Hamiltonian giving us a simpler understanding of the problem. The results in the sd-shell also indicated such a simplification [13].

2. Methods of spectral distribution theory

In spectral distribution theory, one observes that with m valence particles coupling to total isospin T, the energy 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. This asymptotic Gaussian nature of the energy eigenvalue density for the realistic Hamiltonians is seen by finding the higher cumulants in each space of large dimension and observing that they are indeed very small. So, the energy intensities $I_{\mathbf{m},T}(E)$, defined as the energy eigenvalue density $\rho_{\mathbf{m},T}$ times the dimension of the configuration space $d(\mathbf{m},T)$ 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

$$I_{m,T}(E) = \sum_{\mathbf{m}} I_{\mathbf{m},T}(E) = \sum_{\mathbf{m}} d(\mathbf{m},T)\rho_{\mathbf{m},T}(E). \quad (2)$$

The group structure of the shell-model space is exploited in spectral distributions to evaluate traces of operators in these spaces and by dividing the traces by their respective dimensionality, one gets the operator averages. For example, in (m,T) spaces one has the $U(\bar{N}/2) \times U(2)$ subgroup of the $U(\bar{N})$ group with $\bar{N}$ being the total number of single-particle states and for the purpose of evaluating the centroids, the isoscalar (one+two)-body interaction Hamiltonian can be expressed in terms of the group scalars, the number operator n and T^2, as

$$H^0_{\mathrm{TE}} = \epsilon^0 n + [n(n+2) - 4T^2]W^0/8 + [3n(n-2) + 4T^2]W^1/8, \quad (3)$$

where TE stands for trace equivalent, ϵ^0 is the averaged isoscalar single-particle energy and W^0 and W^1 are the averaged two-body isoscalar matrix elements with isospin 0 and 1 respectively. Like the expression for the one-body isoscalar is $\epsilon^0 n$, the isovector one-body is given by $\epsilon^1 \vec{T}$. The isotensor two-body involves the operator $(\vec{T} \times \vec{T})^2$. For extension of the expressions to configuration-isospin spaces as well as for the expressions of widths in these spaces we refer to French [14], Kar [15] and Gomez *et al* [12]. The case of the product of two operators is handled by doing a unitary group decomposition of the spaces and constructing the scalars that survive the evaluation of traces [7]. Alternatively, one looks at spaces with fixed values of neutron and proton numbers, evaluates traces first in the configuration-pn spaces and then generates the traces or averages in configuration-$(\mathbf{m},T)$ spaces through a subtraction procedure [13,16,17].

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 known as the Ratcliff procedure [18]. 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

$$\sum_{\mathbf{m}} \int_{-\infty}^{\bar{E}_i} I_{\mathbf{m},T}(E)\mathrm{d}E = \sum_{k=1}^{i-1} d_k + d_i/2. \quad (4)$$

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 cases $m = 3, T = 1/2$; $m = 5, T = 1/2$; $m = 6, T = 1$ with ^{40}Ca as the closed core, using the fp-shell FPV interaction [19]. These calculations are constrained to have only one particle outside the $0f_{7/2}$ orbit following ref. [2], table 1 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 four orbits to the proton–neutron form in 8 orbits (4 proton orbits plus 4 neutron orbits). The expressions for the pp, nn and pn/np matrix elements for the isoscalar interactions are well known [16] and those for the isovector and isotensor interaction are given by Ormand and Brown [2] and discussed by Kar and Sarkar [13].

Table 1. Centroids and widths of the isoscalar Hamiltonian compared to the centroids and widths of the total Hamiltonian (including the isovector and isotensor parts) in the fixed-T configurations with 3 particles with $T = 1/2, 5$ particles with $T = 1/2$ and 6 particles with $T = 1$ in $0f - 1p$ shell. 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 particles in orbit $1p_{1/2}$.

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 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. (10) of ref. [20]. The numbers in 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 $5/2$ whereas the other three are ground states.

(m, T, J)	LSE for $H^{(0)}$ (MeV)	LSE for total H (MeV)	LSE for $H^{(0)} + H^{(1)}$ (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

3. Results and discussions

Table 1 gives the centroids and widths in all the four 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 (LSE) with the isoscalar plus isovector Hamiltonian $(H^{(0)} + H^{(1)})$ and only the isoscalar Hamiltonian $(H^{(0)})$ to bT_z. The contribution of the Coulomb term to b can be evaluated by using eq. (25) of Lam *et al* [3]. However, in this work we use for b coming from Coulomb energy, the expression given by eq. (10) in the work of Ormand [20] which is a global fit with good accuracy. The experimental values are as quoted in Ormand and Brown [2]. For the 5 particle case along with $J = 7/2$ ground state, the table also presents the values for the first and second excited states with $J = 3/2$ and $5/2$, respectively. We find good agreement between our results and experimental values, keeping in mind that spectral distribution theory is constructed to describe the statistically averaged global properties of nuclei.

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

Table 3. Comparison of $|b|$ using isoscalar with only one-body isovector Hamiltonian with $|b|$ from the full H.

A	T	$\|b\|$ by spectral distributions	$\|b\|$ by spectral distributions with isoscalar and one-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

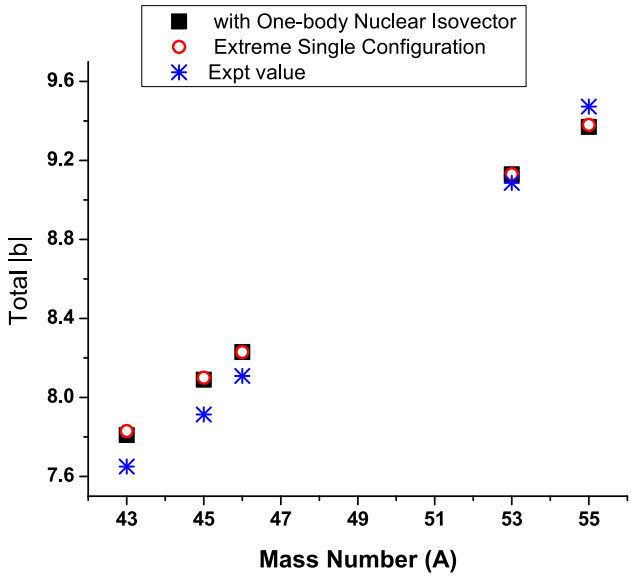

Figure 1. The parameter $|b|$ calculated with only the one–body part of $H^{(1)}$ along with the extreme single configuration estimate for the nuclear part (where all the valence particles are put in the $0f_{7/2}$ orbit) compared to the experimental values for nuclei in the lower part of the fp-shell.

for the sd-shell nuclei in the earlier work of Kar and Sarkar [13].

This originates from the fact that 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]. As the one-body part of the isovector interaction Hamiltonian is just $\epsilon^1 \vec{T}$, one realises that the value of $|b|$ from nuclear interactions is equal to ϵ^1 only. Its configuration-averaged value in spectral distributions is the one averaged by the intensity of each configuration as appearing in our eq. (2). In figure 1 we compare this $|b|$, with the Coulomb part added, against observed values as a function of A for nuclei in the lower half of the fp-shell. For all the cases considered, the dominant configuration is the one where all the particles are in the $0f_{7/2}$ orbit. In the figure we also show the extreme single configuration estimate where the nuclear $|b|$ is equal to $\epsilon^1_{7/2}$, the single-particle matrix element of $H^{(1)}$ for the $0f_{7/2}$ orbit. The configuration-averaged values are seen to be very close to the extreme single configuration estimate. From these results, it appears that an improved agreement with the data for the A dependence of b should come from a better parametrisation of the Coulomb term. 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.

4. Conclusion

In conclusion, we observe that the spectral distribution theory can be used to calculate the energies of the low-lying nuclear states for the Hamiltonian where the isospin non-conserving isovector and isotensor parts are added to the isoscalar part. Then the linear term in the isobaric mass-multiplet equation for isospin-breaking can be calculated from these results 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. We further show that for the calculation of the parameter b, it is a good approximation to retain only the one-body term in the isovector nuclear Hamiltonian.

Acknowledgements

The authors acknowledge Prof. M Saha Sarkar of Saha Institute of Nuclear Physics, Kolkata and Arkabrata Gupta of IIEST, Shibpur for their help during manuscript preparation in LaTeX.

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