Isobaric Multiplet Mass Equation within nuclear Density Functional Theory

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We study Isobaric Multiplet Mass Equation (IMME) within the extended nuclear Density Functional Theory (DFT) that includes isospin-symmetry-breaking (ISB) contact terms and proton-neutron mixing in the particle-hole channel. We focus on isobaric triplets in light nuclei and we delineate contributions to isovector and isotensor IMME coefficients coming from the electromagnetic, isoscalar, and ISB terms of the functional. We compare the DFT results to the available ab initio calculations, so as to evaluate and quantify the role of many-body ISB contributions. The aim is to elucidate the origins of the ISB effects in finite nuclei and to attempt disentangling effects of the strong and Coulomb forces.

Similarity between the neutron-neutron, proton-proton, and proton-neutron nuclear interactions was well recognized already in the third decade of the last century. This property motivated Heisenberg and Wigner to introduce the concept of isospin symmetry, which abandons notions of protons and neutrons and replaces them by that of a nucleon, that is, a particle having two independent states in an abstract space called isotopic-spin space or, in short, the isospace.

The isospin symmetry is not an exact symmetry of nature. At the fundamental level, it is violated by the difference in masses of the constituent up and down quarks and the difference in their electric charges. At the many-body level, where nucleons are treated as structureless point-like particles interacting via the effective forces, the major source of the isospin symmetry breaking (ISB) is the Coulomb field. The strong-force ISB components are much weaker than the symmetry conserving, isoscalar ones. Nevertheless, they are firmly established from the two-body scattering data, which indicate that the neutron-neutron interaction is \( \sim 1\% \) stronger than the proton-proton one, and that the neutron-proton interaction is \( \sim 2.5\% \) stronger than the average of the former two.

Following the classification introduced by Henley and Miller, components of the nuclear force can be divided into four classes that have different structures with respect to the isospin symmetry. Apart from the dominant class-I isoscalar (isospin-invariant) forces, the classification introduces three different classes of the ISB forces, namely, class-II isotensor forces, which break the isospin symmetry but are invariant under a rotation by \( \pi \) with respect to the \( y \)-axis in the isospace; class-III isovector forces that break the isospin symmetry but are symmetric under interchange of nucleonic indices in the isospace, and class-IV forces, which break the isospin symmetry and, in addition, they mix the total isospin. This classification is commonly used in the framework of potential models based on boson-exchange formalism, like CD-Bonn or AV18. It is a convenient point of reference for the effective field theory.

The nuclear density functional theory (DFT), on the other hand, is typically based on isoscalar (class-I) strong forces, with inclusions of class-III forces already proposed in. Only very recently, we have introduced the class-II and class-III contact forces simultaneously. To treat the class-II forces, we employed the local DFT framework involving the proton-neutron mixing.

The isospin symmetry is widely used in theoretical modelling of atomic nuclei. The reason is that the isospin impurity, a measure of the ISB effect in nuclear wave function, is small in heavy \( N = Z \) systems of the order of a few percent. Hence, the isotopic-spin quantum number \( T \) is almost perfectly conserved, and thus it can be used to classify nuclear many-body states and to work out selection rules for nuclear reactions. Although they stem from small components of nuclear wave functions, the ISB effects manifest themselves very clearly in binding energies (BE < 0) of isobaric multiplets. This can be visualized by analyzing the mirror (MDE) and triplet (TDE) displacement energies:

\[
\text{MDE} = \text{BE}(T, T_z = -T) - \text{BE}(T, T_z = +T) \quad \text{and} \quad \text{TDE} = \text{BE}(T, T_z = -1) + \text{BE}(T, T_z = +1) - 2\text{BE}(T, T_z = 0),
\]

respectively. In our previous work, through the analysis of the MDE and TDE binding-energy indicators, we were able to identify and quantify effects related to the ISB class-III and class-II forces, respectively.

In this work, we present a systematic study of the Isobaric Multiplet Mass Equation (IMME):
In this expression also motivates the following IMME variant: the nuclear Coulomb energy can be written as:

\[ \tilde{V}_C = \sum_{\lambda=0}^{2} \tilde{V}_{C,\lambda}. \]  

(2)

Axial components in Eq. (2) reflect the \( T_z \) conservation. Then, with the aid of Wigner-Eckart theorem, the nuclear Coulomb energy can be written as:

\[
\langle \xi, A, T, T_z | \tilde{V}_C | \xi, A, T, T_z \rangle = \langle \xi, A, T | | \tilde{V}_{C,0} | \xi, A, T \rangle \\
\frac{3T_z^2 - T(T + 1)}{\sqrt{T(T + 1)}} \langle \xi, A, T | | \tilde{V}_{C,1} | \xi, A, T \rangle \\
\frac{3T_z^2 - T(T + 1)}{\sqrt{(2T - 1)(T + 1)(2T + 3)}} \langle \xi, A, T | | \tilde{V}_{C,2} | \xi, A, T \rangle. \]  

(3)

This expression also motivates the following IMME variant:

\[ BE(\xi, A, T, T_z) = \sum_{n \leq 2T} a^{(n)}_{A,T,I} Q_n(T, T_z), \]  

(4)

where \( Q_0 = 1, Q_1 = -T_z, \) and \( Q_2 = \frac{1}{2} (3T_z^2 - T(T + 1)) \) are orthogonal isospin polynomials projecting the isoscalar, isovector \( I^+ \) and isovector components, respectively, see Ref. [21]. Obviously, the two variants 11 and 14 are fully equivalent, with \( a = a^{(0)}_{A,T,I} + \frac{1}{2} T(T + 1)a^{(2)}_{A,T,I}, \) \( b = -a^{(1)}_{A,T,I}, \) and \( c = \frac{3}{2} a^{(2)}_{A,T,I}. \) Moreover, had they been exact, we would have the displacement energies of MDE = \(-2Tb\) and TDE = \(2T^2c.\) Of course, for triplets \((T = 1),\) nuclear masses can always be trivially described by a parabolic dependence on \( T_z,\) so in our work, we rather address the question of a microscopic derivation of IMME coefficients \( b \) and \( c.\) For higher multiplets \((T > 1),\) there is an active ongoing debate if higher-order terms, \(dT_3^2\) or \(dT_3^4,\) are required, see Refs. [22, 23] for brief recent reviews.

Our study is based on the recently developed extended single-reference Skyrme DFT that includes proton-neutron mixing in the particle-hole channel [13, 16] and zero-range class-II and class-III contact forces with the coupling constants adjusted to reproduce available data on MDEs and TDEs in \( A \geq 10 \) nuclei [14]. Here we focus on investigating the intrinsic structure of the IMME coefficients \( b \) and \( c \) in isospin triplets, by decomposing them into contributions coming from the electromagnetic, contact ISB, and isoscalar parts of the functional. By comparing the DFT results with those obtained using the \( ab \) initio methods in \( A = 8 \) and \( A = 10 \) triplets, see Refs. [21, 22], we attempt to bridge our phenomenological ISB forces having low-energy coupling constants (LECs) fitted to many-body data to the AV18 [4] ISB \( ab \) initio forces having LECs adjusted to two-body scattering data. Such a comparison provides us with clues concerning a possible role of the (diagonal) three- and higher-body ISB effects, which, if exist at all, enter our formalism through the fit to heavy nuclei.

The extended DFT involves the Coulomb force, conventional isoscalar Skyrme interaction, and the following zero-range interactions of class II and class III [14]:

\[
\hat{V}^{\text{II}}(i,j) = t^{\text{II}}_0 \delta(r_i - r_j) \left[ 3\hat{r}_3(i)\hat{r}_3(j) - \hat{r}(i) \circ \hat{r}(j) \right], \]  

(5)

\[
\hat{V}^{\text{III}}(i,j) = t^{\text{III}}_0 \delta(r_i - r_j) \left[ \hat{r}_3(i) + \hat{r}_3(j) \right]. \]  

(6)

Hence, the extended formalism depends on two new LECs, \( t^{\text{II}}_0 \) and \( t^{\text{III}}_0.\)

Our extension of the standard Skyrme DFT to ISB forces was implemented within the code HFDDD (v2.73y) [20] that allows for the proton-neutron mixing – another angle of the cranking technique, which is widely used in high-spin physics. The method allows us to calculate the entire isospin multiplet, \( T, \) by starting from the \( z \)-aligned state \( |T, T_z = T \rangle \) and isocranking it around the axis tilted by angle \( \theta \) in the isospace [14]. Calculations for the \( A = 8, \ldots, 58 \) triplets, which we discuss below, were performed using the coupling constants derived in Ref. [14], that is, for \( t^{\text{II}}_0 \) equal to \( 4.6 \pm 1.6, 7 \pm 4, \) and \( 6 \pm 4 \) MeV fm\(^3\) for the SV\(^3\)\text{IB}, SkM*\text{ISB}, \) and SLy\(^4\)\text{ISB} functional, respectively, and for \( t^{\text{III}}_0 \) respectively equal to \(-7.4 \pm 1.9, -5.6 \pm 1.4, \) and \(-5.6 \pm 1.4 \) MeV fm\(^3\).

To obtain a deeper insight into the nature of the strong-force ISB mechanism, one has to compare the DFT results obtained for the ISB-sensitive many-body (pseudo)observables to those given by \( ab \) initio methods. To this end, we performed systematic studies of the isovectorial and isoscalarial IMME coefficients in light \( A = 8, 10, 12, \) and 14 isospin triplets. The extended DFT results can then be directly compared to the Green Function Monte Carlo (GFMC) results, which are, at present, available for the isospin triplets in \( A = 8 \) and 10 nuclei, see Refs. [6, 24]. The comparison was separately performed for the electromagnetic, ISB, and isoscalar \((T = 0)\) contributions to the IMME coefficients.

This method allows for a quantitative assessment of different contributions to the ISB effect. Such comparison is particularly valuable, because the ISB sectors in the DFT and GFMC differ. The GFMC calculations involve the high-precision potential AV18 [3, which takes into account ISB effects due to the one-photon and higher-order electromagnetic effects, isovector kinetic energy, and class-II and class-III strong finite-range regularized interactions. In Refs. [7, 27] the potential was further generalized to include also class-IV strong force. On the other hand, our DFT modelling captures all ISB effects (beyond the mean-field Coulomb) in two LECs corresponding to contact-class II and class-III forces.

The DFT and GFMC results are collected in Tables [11] and [11]. Calculated coefficients \( a^{(1)}_{A,T,I} \) and \( a^{(2)}_{A,T,I} \) are de-
TABLE I. Contributions of the electromagnetic ($V^\gamma$), ISB nuclear ($V^{\text{ISB}}$), and isoscalar ($H^\text{T=0}$) forces to coefficients $a_{A,T,I}^{(1)}$, see Eq. (4), in the $A = 8$ and $A = 10$ triplets, calculated using the GFMC and the extended DFT models. Theoretical uncertainties of the adjusted coefficients are of similar quality, but also lead to similar individual contributions coming from electromagnetic and ISB forces. This may suggest that the ISB effects related to the electromagnetic correlations beyond mean-field, included and not included in the ab initio and DFT calculations, respectively, do not dominate in the physical picture.

| Model   | $V^\gamma$ | $V^{\text{ISB}}$ | $H^\text{T=0}$ | Total | EXP  |
|---------|------------|-----------------|----------------|-------|------|
| GFMC    | 1675(1)    | 102(1)          | 43(6)          | 1813(6)| 1770 |
| SV_T    | 1729       | 370             | 20             | 2119(96)|      |
| GFMC    | 2155(7)    | 110(1)          | —              | 2170(8)| 2329 |
| SV_T    | 2152       | 355             | 28             | 2535(92)|      |
| SV_T    | 2588       | 421             | 34             | 3043(109)| 2767 |
| SV_T    | 3004       | 490             | 38             | 3532(127)|      |

TABLE II. Same as in Table I but for coefficients $a_{A,T,I}^{(2)}$.

| Model   | $V^\gamma$ | $V^{\text{ISB}}$ | $H^\text{T=0}$ | Total | EXP  |
|---------|------------|-----------------|----------------|-------|------|
| GFMC    | 136(1)     | 3(2)            | 10(5)          | 139(5) | 127  |
| SV_T    | 145        | 27              | 11             | 183(8) |      |
| GFMC    | 178(1)     | 119(18)         | —              | 297(19)| 241  |
| SV_T    | 155        | 118             | 11             | 284(43)|      |
| SV_T    | 134        | 24              | 8              | 166(10)| 162  |
| SV_T    | 143        | 83              | 7              | 233(31)| 225  |

FIG. 1. (Color online) (Left) The IMME coefficients $a_{A,T,I}^{(1)}$ (a) and $a_{A,T,I}^{(2)}$ (b), see Eq. (4). Experimental values are labeled by diamonds. Full and open circles mark our DFT results calculated using the SV_T and SV_T functional, respectively. Squares label the GFMC values taken from [22]. (Right) Contributions to the IMME coefficients $\delta a_{A,T,I}^{(1)}$ (c) and $\delta a_{A,T,I}^{(2)}$ (d) due to electromagnetic and isoscalar forces (open symbols) and ISB forces (full symbols). The DFT and GFMC results are labeled by circles and squares, respectively. The GFMC ISB contributions include also those due to the isovector kinetic energy.

tions to $a_{A,T,I}^{(1)}$ due to the leading-order electrostatic contributions but differ considerably concerning the subleading nuclear ISB contributions, see Fig. (1c) and Tables I and II. The DFT ISB contribution to $a_{A,T,I}^{(1)}$ is roughly three times larger than the corresponding GFMC result.

The isotensorial coefficients $a_{A,T,I}^{(2)}$, on the other hand, are very well reproduced by both models. This holds for both the total values, see Fig. (1b), and individual contributions due to electrostatic and ISB effects, see Fig. (1d). In the DFT calculations, the staggering in $a_{A,T,I}^{(2)}$, Fig. (1d), comes entirely from the contact class-II force. More precisely, it is due to the class-II time-odd mean-field as shown in Fig. (2a). In the ab initio calculation both the electrostatic as well as the strong class-II force contribute to the staggering, but the latter contribution prevails.

The comparison presented in Fig. (2) allows us to draw the main conclusions of this Letter. Indeed, the ab initio and DFT results not only reproduce the total values of the IMME coefficients in a similar way, but also lead to similar individual contributions coming from electromagnetic and ISB forces. This may suggest that the ISB effects related to the electromagnetic correlations beyond mean field, included and not included in the ab initio and DFT calculations, respectively, do not dominate in the physical picture.

Recently, Ormand et al. [10] performed seminal ab initio study of the isotensorial coefficients $c^{(1)}$ in the $pf$-
Fig. 3, for the experimental values of the deformation, in Table III and have a profound impact on cences influence rather weakly the calculated weakly deformed shapes. It appears that shape differ-

ence, those for SkM* SV

triplets using generalized DFT approach that includes electrostatic, ISB, and isoscalar contributions to the isotensorial coefficients. The total IMME coefficients and par-

triplets, the SV

In conclusion, we performed systematic study of isovec-

We showed that the DFT calculations involving SV

functional and the GFMC calculations reproduce empirical a(1) and a(2) coefficients comparably well. The Coulomb contributions to the isovector a(1) and isoten-

soor

and so are the contributions to a(2) coefficient due to the ISB effects. The ISB contribution to a(1) is almost three time larger in the DFT as compared to the GFMC. Both models associate the staggering pattern in a(2) with ISB effects. In

shell A=42, 46, 50, and 54 isospin triplets. Their results systematically overestimate the experimental values, irrespective of which high-precision ab initio potential, CD-Bonn [3], AV18 [1], or N3LO [3], is used in the calculations, see Fig. 2(b). Conversely, our DFT calculations underestimate the experimental data. The individual contributions to the isotensorial coefficients c due to the electrostatic and ISB forces also differ.

For isospin triplets in 8 ≤ A ≤ 58 nuclei, we performed systematic calculations of the IMME coefficients b and c, Eq. 1, using three different functionals: SV

T

and isoscalar contributions due to electrostatic, ISB, and isoscalar terms in the functional were compared to the existing GFMC calculations in A=8 and 10 isobaric triplets.

TABLE III. Calculated DFT IMME coefficients b and c, Eq. 1 and their uncertainties Δb and Δc, respectively. For A > 8, we show values of averaged over the results obtained for the SV

T

and SLy4 ISB functional, and for A = 8 those corresponding to SV

T

only. Theoretical uncertainties Δ were estimated according to the methodology presented in [15]. All values are in MeV.

| A   | b   | Δb  | c   | Δc  |
|-----|-----|-----|-----|-----|
| 8   | −2.11 | 0.10 | 0.19 | 0.02 |
| 10  | −2.56 | 0.08 | 0.43 | 0.05 |
| 12  | −2.96 | 0.11 | 0.30 | 0.06 |
| 14  | −3.35 | 0.18 | 0.34 | 0.05 |
| 16  | −3.64 | 0.11 | 0.24 | 0.06 |
| 18  | −3.90 | 0.08 | 0.33 | 0.05 |
| 20  | −4.31 | 0.08 | 0.30 | 0.05 |
| 22  | −4.64 | 0.08 | 0.30 | 0.05 |
| 24  | −4.99 | 0.09 | 0.22 | 0.05 |
| 26  | −5.35 | 0.10 | 0.29 | 0.05 |
| 28  | −5.68 | 0.10 | 0.21 | 0.05 |
| 30  | −5.98 | 0.11 | 0.31 | 0.06 |
| 32  | −6.22 | 0.08 | 0.28 | 0.05 |

For A > 8 over the results obtained for the three functionals, are collected in Table III along with their theoretical uncertainties, and plotted in Fig. 3 For all three functionals, the calculated coefficients b, and c for A > 8, have similar values. However, for the A = 8 triplet, the SV

T

calculations lead to a ground state having well deformed prolate shape (β2 ≈ 0.38). At variance, those for SkM* ISB and SLy4 ISB converge to oblate, weakly deformed shapes. It appears that shape differences influence rather weakly the calculated b values but have a profound impact on c. Therefore, to comply with experimental values of the deformation, in Table III and Fig. 4 for the A = 8 triplet we show the unaveraged SV

T

results.

In conclusion, we performed systematic study of isovector and isotensor IMME coefficients in light isobaric triplets using generalized DFT approach that includes contact ISB forces. The total IMME coefficients and partial contributions due to electrostatic, ISB, and isoscalar terms in the functional were compared to the existing GFMC calculations in A=8 and 10 isobaric triplets.

FIG. 3. (Color online) Calculated DFT IMME coefficients b (a) and c (b) of Table III plotted in comparison with experimental results derived from binding [21] and excitation [22] energies. Shaded areas indicate values of estimated theoretical uncertainties.

FIG. 2. (Color online) (Left) Contributions to the DFT IMME coefficient δA,T,I (2) due to time-even (full symbols) and time-odd (open symbols) class-II (up triangles) and class-III (down triangles) ISB components. (Right) Isotensor coefficient c of the IMME variant. Diamonds represent experimental data and full circles with error bars mark our DFT results. Up triangles, squares, and down triangles label the results obtained in Ref. [10] using, respectively, the CD-Bonn, AV18, and N3LO high-precision ab initio potentials at 3rd order.
the DFT calculations, the effect is almost entirely due to time-odd class-II mean-field.

We also showed that the DFT calculations involving SV\textsubscript{ISB} functional underestimate the isoscalar coefficients in $A=42, 46, 50,$ and $54$ pf-shell nuclei, at variance to the recent ab initio calculations of Ref. [10], which overestimate the experiment irrespective of the ab initio potential being used. These two methods predict also very different contributions to $c$ due to the Coulomb and ISB forces. However, results of Ref. [10] do not seem yet to converge with respect to the order of the calculation, and the results corresponding to the $A = 4n$ triplets are not yet available. The DFT results presented in this Letter may thus serve as a baseline for future comparisons in heavy nuclei.

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