Invited Comment

Isospin effects in $N \approx Z$ nuclei in extended density functional theory

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Received 12 October 2015, revised 27 December 2015
Accepted for publication 8 January 2016
Published 25 January 2016

Abstract

This paper overviews various phenomena related to the concept of isospin symmetry. The focus is on $N \approx Z$ nuclei, which are excellent laboratories of isospin physics. The theoretical framework applied is nuclear density functional theory and its isospin- and angular-momentum projected extensions, as well as symmetry-projected multi-reference models. The topics covered include: isospin impurities, superallowed Fermi beta decays, beta-transitions in mirror nuclei, isospin breaking hadronic interactions, mirror and triplet binding energy differences, and isoscalar pairing.

Keywords: isobaric spin, nuclear density functional theory and extensions, effective interactions, beta decay, nuclear tests of fundamental interactions and symmetries

(Some figures may appear in colour only in the online journal)

1. Introduction

Isobaric spin was introduced by Heisenberg [1] in order to explain the neutron–proton (np) symmetry. Subsequently, the isospin symmetry has been widely used in theoretical modeling of the atomic nuclei [2–4]. Even though it is broken by the electroweak force, isospin is extremely useful for our understanding of nuclear structure and decays.

Of particular interest for isospin physics are $N \approx Z$ nuclei. Beyond the Ca, many of them are located far from the line of beta stability, in close proximity to the proton drip line. Because of the similarity of proton and neutron shell-model orbits, the $N \approx Z$ systems exhibit unique phenomena related to the attractive nature of the isoscalar component of the nuclear force. Examples are: superallowed Fermi beta decays [5], superallowed Gamow–Teller (GT) decays [6], superallowed alpha decays [7], Wigner energy [8], isoscalar pairing [9], and collective modes [10].

The atomic nuclei with enhanced sensitivity to fundamental symmetries are unique laboratories to search for signals of new physics beyond the standard model. The $N \approx Z$ nuclei are particularly interesting probes as the superallowed $I = 0^+ \rightarrow I = 0^+$ beta-decays among the isobaric analogue states in the isospin triplet allow stringent tests of the conserved vector current (CVC) hypothesis and provide precise values of the strength of the weak force and the leading $V_{ud}$ element of the Cabibbo–Kobayashi–Maskawa matrix. Other examples include Fermi- and GT ground-state (g.s.) beta-decays in $T = 1/2$ mirror nuclei, which offer alternative tests of the electroweak sector. In all these cases, high-fidelity theoretical calculations of radiative corrections and isospin symmetry breaking (ISB) effects are needed to extract the crucial information from precise measurements.

The theory roadmap for this area involves ab initio and configuration interaction (shell model) approaches, and nuclear density functional theory (DFT). The latter is the tool of choice for open-shell, deformed complex systems. The focus of this paper is on DFT-based frameworks and their extensions, including multi-reference approaches involving symmetry restoration. Such models are able to capture core-polarization effects originating from a subtle interplay between the long-range Coulomb interaction and short-range
2. Isospin impurity

The degree of isospin symmetry violation—the isospin impurity—is a result of a subtle balance between the attractive short-range strong force and the repulsive long-range Coulomb interaction that polarizes the entire nucleus. Consequently, its precise theoretical treatment requires the use of a no-core framework which, in heavier nuclei, is provided by nuclear DFT.

The early attempts to evaluate the degree of isospin breaking, measured in terms of the isospin impurity \( \alpha_C \), date back to the 1960s, see [11] for a review. These estimates, based on perturbation theory [12] or analytically solvable hydrodynamical model [13], were able to explain some gross features of \( \alpha_C \) such as the steady increase of isospin mixing along the \( N - Z \) line with increasing \( A \) or quenching of \( \alpha_C \) with increasing \( |N - Z| \). These early models, however, were not too quantitative.

The accurate calculation of the isospin impurities has been challenging. This was early realized by Engelbrecht and Lermer [18] who pointed out that the self-consistent mean-field (MF) approaches cannot be directly applied because of the spurious mixing caused by the spontaneous ISB effects. To eliminate the problem of spurious admixtures in the wave function, we have developed a no-core MR-DFT model involving isospin projection, see also [19, 20]. The model employs self-consistent, isospin-broken MF states \( |\varphi\rangle \). Self-consistency is needed to ensure that the balance between the Coulomb force and the strong interaction, represented in our model by the Skyrme energy density functional (EDF), are properly taken into account. The MF state can be formally decomposed into good-isospin basis \( |T, T\rangle \):

\[
|\varphi\rangle = \sum_{T \geq |T|} b_{T,|T|} |T, T\rangle, \quad \sum_{T \geq |T|} |b_{T,|T|}|^2 = 1, \tag{1}
\]

where \( T \) and \( T = (N - Z)/2 \) are the total isospin and its third component, respectively. The mixing coefficients \( b_{T,|T|} \) can be calculated using the states

\[
|T, T\rangle = \frac{1}{\sqrt{|NTT|}} \hat{P}_T |\varphi\rangle \tag{2}
\]

obtained by isospin projection after variation.

To assess the isospin mixing, one has to rediagonalize the total Hamiltonian \( \hat{H} \) involving strong interaction plus the Coulomb term in the space spanned by the good-isospin basis (2):

\[
|n, T\rangle = \sum_{T \geq |T|} a_{nT,|T|}^T |T, T\rangle, \tag{3}
\]

where \( n \) enumerates the eigenstates \( |n, T\rangle \) of \( \hat{H} \). The value of \( n = 1 \) corresponds to the isospin-mixed g.s. The g.s. isospin-mixing parameter obtained after rediagonalization (AR) is defined as:

\[
\alpha_C = 1 - |a_{1T,|T|}^T|^2. \tag{4}
\]

Comparison of \( \alpha_C \) with the quantity \( \alpha_C^{(BR)} = 1 - |b_{1T,|T|}|^2 \) obtained before rediagonalization (BR) provides direct information about the spuriousity of MF solutions. As shown in figure 1, the isospin impurities exceed MF values by almost 30%.

The empirical information on isospin impurities in heavier systems is both scarce and uncertain. The values of \( \alpha_C \) extracted from a forbidden E1 transition in \( ^{64}\text{Ge} \) or from the decay of giant dipole resonance in \( ^{90}\text{Zr} \) are consistent with the predictions of the isospin-projected DFT but the experimental uncertainties are too large to discriminate between different EDF parameterizations. Indeed, as shown in figure 2, the spread in \( \alpha_C \) obtained with nine Skyrme EDFT, \( \alpha_C \approx 4.4\% \pm 0.3\% \), is relatively small and lies well within the experimental uncertainty limits. The figure shows the calculated impurities versus excitation energy \( \Delta E_{T=1} \) for the lowest \( T = 1 \) state in even-even \( N = Z \) nuclei, which is referred to as the doorway state. It is seen that the larger excitation energy of the doorway state the smaller impurity, with exception of the SkO’ result.
Figure 3 shows the calculated excitation energy of the doorway state for the three Skyrme EDFs: SIII, SLy4, and SkP. Filled (open) circles refer to AR (BR) results, respectively. The AR results lie within experimental uncertainty limits of [16] while the BR values are ruled out by the data. (Taken from [21].)

**Figure 3.** Excitation energies of the doorway states $E_{\text{T}=1}$ in the even-even $N = Z$ nuclei relative to the g.s. energies $E_{\text{HF}}$ obtained with SIII (diamonds), SLy4 (dots), and SkP (circles) Skyrme EDFs. Horizontal lines mark the mean values. The estimates based on the perturbation theory [12] and the hydrodynamical model [13] are indicated by thick dotted lines. (Adopted from [24].)

Excitation energies of the doorway states and, in turn, isospin impurities, depend on EDF parameterization. It is, however, not at all obvious what EDF components are responsible for the systematic differences seen in figure 3. Indeed, attempts to correlate $\alpha_C$ with various bulk properties of Skyrme EDFs turned out to be fairly inconclusive. For example, no correlation has been found with the symmetry energy [25], which is the primary quantity characterizing the isovector properties of EDFs. As illustrated in figure 4, no clear correlation has been found between $\alpha_C$ and the isovector and isoscalar effective mass.

We do find, however, a strong correlation between $\alpha_C^{(BR)}$ and the proton skin, i.e., the difference between proton and neutron root mean square radii, see figure 5 and [26]. The correlation deteriorates for $\alpha_C^{(AR)}$, indicating again that the isospin mixing is a non-perturbative quantity; hence difficult to estimate.
The formalism discussed above can be extended to incorporate the angular-momentum projection. In this case, the basis is created by applying the isospin \( \hat{P}_T \) and angular-momentum \( \hat{P}_{MK} \) projection to \( |\psi\rangle \):

\[
|I, M; K; T, T_z\rangle = \frac{1}{\sqrt{N_{Tz,1MK}}} \hat{P}_{Tz} \hat{P}_{MK} |\psi\rangle,
\]

where \( M \) and \( K \) denote the magnetic quantum numbers associated with the laboratory and intrinsic \( z \)-axes, respectively [27]. Because \( K \) is not conserved, the set (5) is overcomplete. This problem can be overcome by rediagonalization of the Hamiltonian in the so-called collective space, spanned for each \( I \) and \( T \) by the natural states, \( |IM; TT_z|^{(i)} \) [28, 29]. The wave functions

\[
|n; IM; TT_z\rangle = \sum_{i,T_z} a_{n,i}^{(0)} |IM; TT_z|^{(i)}
\]

obtained in the rediagonalization are labeled by the index \( n \) and conserved quantum numbers \( I, M, \) and \( T_z \).

The double-projected and isospin-projected approaches yield very similar g.s. isospin impurities in even-even nuclei. However, there are configurations for which the model solely relying on isospin projection is insufficient. Among them there are the so-called anti-aligned configurations in odd-odd \( N = Z \) nuclei, which are crucial for calculations of ISB corrections to the superallowed beta-decay involving the \( T = 1 \), \( J = 0^+ \) states in odd-odd nuclei. These states are not representable by a single MF configuration as shown schematically in figure 6. Indeed, the odd proton and odd neutron can form either the aligned or anti-aligned configuration. The aligned configuration represents an isoscalar \( T = 0 \), \( J = 0^\circ \) state. The anti-aligned configuration, however, manifestly breaks the isospin symmetry being an equal mixture of isoscalar and isovector states. The calculations indicate [30] that the \( T = 0 \) and \( T = 1 \) components projected from the anti-aligned configuration strongly mix through the Coulomb interaction leading to unphysically large isospin impurities. Double-projected approach is free from such pathologies. This is demonstrated in the lower part of figure 7 for a representative case of \( ^{42}\text{Sc} \).

It can be shown [24] that the isospin projection technique can be safely used within nuclear DFT. Augmenting the isospin projection with the angular-momentum projection leads to a number of theoretical issues. Not only the numerical complexity of computations increases but also the uncontrolled singularities appear in the energy kernels [21]; this essentially eliminates a possibility to use modern EDFs with density-dependent terms [31]. To overcome this problem, regularization schemes have been proposed [32, 33] but they are difficult in practical implementations. Until a workable solution is developed, a practical option is to use Hamiltonian-based EDFs, such as the SV force [22] augmented by the tensor terms, or the recently developed SLyMR forces that include three- and four-body terms [34].

All the existing parameterizations of the density-independent Skyrme EDF are characterized by a nonstandard saturation mechanism driven by a very low isoscalar effective mass \( m^*_S \approx 0.4 \). The low effective mass affects the overall performance of those forces, impairing such key properties as the symmetry energy, level density, and level ordering. The low value of \( m^*_S \) also impacts the isospin mixing. In particular, in the case of \(^{88}\text{Zr} \) discussed above, the SV EDF yields \( \alpha_C \approx 2.8\% \), which is considerably smaller than the mean value, \( \bar{\alpha}_C \approx 4.4 \pm 0.3\% \), obtained by averaging over the EDFs shown in figure 2. The lack of a reasonable Hamiltonian-based Skyrme EDF is probably the most critical deficiency of the current self-consistent approach. Nonetheless, one has to admit that the EDFs with low effective masses perform surprisingly well when used in the context of no-core-configuration-interaction (NCCI) extensions [35–38].

Figure 6. Left: schematic illustration of two possible mean-field g.s. configurations in an odd-odd \( N = Z \) nucleus. Upper (lower) configuration is called aligned (anti-aligned). Right: the result of the isospin symmetry restoration. The aligned configuration is isoscalar; hence, it is insensitive to the isospin projection. The anti-aligned configuration represents a mixture of \( T = 0 \) and \( T = 1 \) states. The projection lifts the isospin degeneracy by lowering the \( T = 0 \) level. (Taken from [30].)

Figure 7. Isospin impurities in \(^{42}\text{Sc} \), calculated for four antialigned configurations \( |\nu K \oplus \pi K\rangle \) obtained by putting the valence neutron and proton in opposite-\( K \) Nilsson orbitals originating from the \( f_{7/2} \) shell. Open and full dots show the results obtained in isospin-projected and double-projected \((I = 0, T = 0)\) variants, respectively. (Adopted from [25].)
3. ISB corrections to the superallowed $J^P = 0^+$, $T = 1 \rightarrow J^P = 0^+$, $T = 1$ beta decays

The superallowed $J^P = 0^+$, $T = 1 \rightarrow J^P = 0^+$, $T = 1$ beta transitions are of particular importance for testing various aspects of the electro-weak sector of the standard model. What makes these pure Fermi decays so useful is the CVC hypothesis, which states that the vector current is not renormalized in the nuclear medium. This implies that the product of the statistical rate function $f$ and partial half-life $t$ for the superallowed $I = 0^+$, $T = 1 \rightarrow I = 0^+$, $T = 1$ Fermi beta-decay should be nucleus-independent and equal to:

$$f t = \frac{K}{G_V \lambda^2(M_F^{(\pm)})^2} = \text{const},$$

(7)

where

$$K/(\hbar c)^6 = \frac{2\pi^3 h}{\lambda^2} \ln 2/\left(m_e c^2\right)^2 = 8120.2787 \times 10^{-10} \text{ GeV}^{-4} \text{s}$$

is a universal constant; $G_V$ stands for the vector coupling constant for semi-leptonic weak interaction; and $M_F^{(\pm)}$ is the nuclear matrix element of the isospin operator $\hat{T}$.  

In reality, the relation (7) holds only approximately and must be slightly amended to account for radiative processes and ISB effects. Fortunately, the radiative and ISB corrections are small, of the order of a few percent, and this allows us to express the rate conveniently as:

$$f t \equiv f t(1 + \delta_R) = \frac{K}{2G_V' \lambda^2(1 + \Delta_R)},$$

(8)

with the left-hand side being nucleus independent. In equation (8), $\Delta_R = 2.36138 + 0.00038$ stands for the nucleus-independent part of the radiative correction [39], $\delta_R'$ is a transition-dependent (Z-dependent) but nuclear-structure-independent part of the radiative correction [39, 40], and $\Delta_{NS}$ denotes the nuclear-structure-dependent part of the radiative correction [40, 41]. The ISB correction $\delta_{ISB}$ is a many-body correction to the nuclear matrix element:

$$|M_F^{(\pm)}|^2 = 2(1 - \delta_{ISB}),$$

(9)

accounting for the isospin-symmetry violation in the atomic nuclei, see [5, 42–45] and references cited therein.

In spite of explicit dependence on theoretical input and the related uncertainties in the calculated radiative and ISB corrections, the superallowed beta-decays provide today’s most accurate value of the vector coupling constant $G_V$. Moreover, they enable a very accurate verification of the CVC hypothesis and provide precise information on the leading matrix element $V_{ud} = G_V/G_{f_{ud}}$ of the CKM three-generation quark mixing matrix [5, 44–48]. This is so because the vector coupling constant, $G_V/(\hbar c)^3 = 1.16637 \times 10^{-5} \text{ GeV}^{-2}$, is well known from the muon decay [48]. The uncertainty of $V_{ud}$ extracted from the superallowed beta-decays is almost by an order of magnitude smaller as compared to the values obtained from neutron or pion decays [48].

In search for physics beyond the standard model, precision is of utmost importance. Only those transitions that have $ft$-values measured with an accuracy $\leq 0.3\%$ are acceptable. The canonical set of transitions used over the last decade to test the standard model consists of 13 such cases spreading over a wide range of masses from $A = 10$ ($^{10}$Ca) to $A = 74$ ($^{38}$Rb), see [4, 44, 45]. With the CVC hypothesis confirmed, it is possible to extract $V_{ud}$ by averaging over several transitions. This feature makes the superallowed beta-decay strategy very attractive. Recently, the canonical set has been extended by a measurement of the beta-decay of $^{38}$Ca [49, 50]. Moreover, the superallowed decay of $^{18}$Ne is within experimental reach [51].

The ISB corrections $\delta_{ISB}$ were computed in diverse nuclear models, see [45, 52–57]. The standard in this field has been set by Hardy and Towner (HT) [5, 40, 43–45] who have used the nuclear shell model (NSM) to account for the configuration mixing effect in conjunction with the MF potential needed to account for a radial mismatch of proton and neutron single-particle (s.p.) wave functions due to the long-range Coulomb polarization [53]. Such a description has certain practical advantages. For instance, it allows for an independent fine-tuning of various model’s ingredients. But it also leads to internal inconsistencies. In particular, the HT model violates the SU(2) commutation rules for the bare isospin operators as pointed out in [58, 59]. Unfortunately, the associated uncertainty is difficult to quantify.

The self-consistent multi-reference DFT involving the isospin- and angular-momentum projections [24, 26, 30, 57] is an interesting alternative to the fine-tuned phenomenological HT approach. This is a no-core theory, which is capable of treating rigorously the rotational symmetry and explicit breaking of isospin symmetry. The correct balance between the Coulomb and hadronic forces is maintained by self-consistency requirements. The approach allows for a rigorous treatment of the Fermi matrix elements using bare isospin operators. The recently proposed NCCI extensions of the framework [36, 37, 60] allow to take into account more correlations due to inclusion of (multi)particle-(multi)hole configurations. As already mentioned, the weakest point of the formalism is the lack of a reasonable Hamiltonian-based Skyrme EDF. One should stress, however, that $\delta_{ISB}$ does not depend on the absolute magnitude of isospin mixing but rather on a difference between parent and daughter states [56], i.e., it is a less sensitive quantity.

The MR-DFT calculations of $\delta_{ISB}$ involving single reference states in parent and daughter nuclei are carried out as follows. The superallowed $0^+ \rightarrow 0^+$ Fermi beta-decay proceeds between the g.s. $|I = 0, T \approx 1, T_z = \pm 1\rangle$ of the even–even nucleus and its isospin-analogue partner $|I = 0, T \approx 1, T_z = 0\rangle$ in the $N = Z$ odd–odd nucleus. The corresponding transition matrix element is:

$$M_F^{(\pm)} = \langle I = 0, T \approx 1, T_z = \pm 1|\hat{T}_z|I = 0, T \approx 1, T_z = 0\rangle.$$  

(10)

Within the MR-DFT, the parent g.s. is approximated by a projected state

$$|I = 0, T \approx 1, T_z = \pm 1\rangle = \sum_{T \geq 1} c_T^{(+)} P_{\pm 1, \pm 1}^{(T)} P_{0,0}^{(0)} |\psi\rangle,$$

(11)
where $|\psi\rangle$ is the g.s. of the even–even nucleus obtained in the self-consistent Hartree–Fock calculations. The state $|\psi\rangle$ is unambiguously defined by filling in the pairwise doubly-degenerate levels of protons and neutrons up to the Fermi level. The daughter state is approximated by

$$|I = 0, T \approx 1, T_z = 0\rangle = \sum_{J \geq 0} \gamma_J \tilde{P}_{u,0,0}^J \tilde{P}_{l=0}^J |\varphi\rangle,$$

(12)

where the self-consistent Slater determinant $|\varphi\rangle \equiv |p \otimes \pi\rangle$ (or $|\nu \otimes \pi\rangle$) represents the anti-aligned configuration, selected by placing the odd neutron and the odd proton in the lowest available time-reversed (or signature-reversed) s.p. orbits. The isospin-projected state shown in figure 6, based on the $|\varphi\rangle$ configuration that manifestly breaks the isospin symmetry, is indeed a preferred way to access the $|T \approx 1, I = 0\rangle$ states in odd–odd $N = Z$ nuclei.

The anti-aligned configurations in odd–odd $N = Z$ nuclei are not uniquely defined. In the signature-symmetry-restricted calculations, there are in general three anti-aligned Slater determinants with the s.p. angular momenta (alignments) of the valence protons and neutrons pointing along the Ox, Oy, or Oz axes of the intrinsic shape defined by means of the long (Oz), intermediate (Ox), and short (Oy) principal axes of the nuclear mass distribution, respectively. Thus far, in spite of persistent efforts, no self-consistent tilted-axis g.s. solutions have been found. Various properties of these linearly dependent solutions, hereafter referred to as $|\varphi_Y\rangle$, $|\varphi_\pi\rangle$, and $|\varphi_2\rangle$, are discussed in detail in [30] and will not be repeated here.

In a MR-DFT double-projection approach based on a single reference state, the only way to deal with the shape-current orientation ambiguity is to calculate three independent beta-decay matrix elements corresponding to each orientation and average over the resulting values of $\delta_C$. Such an strategy was adopted in [30], which contains the calculated corrections for the canonical set of superallowed transition as well as predictions for yet-unmeasured cases. The calculated corrections are in reasonable agreement with the HT results as shown in figure 8. Both sets of corrections systematically overestimate the RPA results of [55].

With the set of ISB corrections obtained in [30], one obtains $\tau = 3073.6(12)$ s, which gives $|V_{\text{ud}}| = 0.973977(27)$. This value is in excellent agreement with the HT result [40], $|V_{\text{ud}}|^{\text{HT}} = 0.97418(26)$, and the central value obtained from the neutron decay, $|V_{\text{ud}}^{\text{n}}| = 0.9746(19)$ [61]. Taking the calculated $|V_{\text{ud}}|$ and combining it with $|V_{\text{ol}}| = 0.2252(9)$ and $|V_{\text{sd}}| = 0.00389(44)$ from the 2010 Particle Data Group [61], one obtains

$$|V_{\text{ud}}|^2 + |V_{\text{ol}}|^2 + |V_{\text{sd}}|^2 = 0.99935(67),$$

(13)

which implies that the unitarity of the first row of the CKM matrix is satisfied with a precision better than 0.1%. A survey of the $|V_{\text{ud}}|$ values obtained using different methods is shown in figure 9.

The solutions $|\varphi_Y\rangle$, $|\varphi_\pi\rangle$, and $|\varphi_2\rangle$, differ by at most a few hundred keV in energy. Hence, there is no obvious preference for a choice of reference state. Moreover, the orientation-dependent effects originate, predominantly, from the time-odd fields of the nuclear MF. Hence, the orientation effects are present only in odd–odd nucleus adding up to a difference between parent and daughter nuclei. The averaging procedure applied in [30] should be considered as a purely practical solution. The shape-current-orientation ambiguity has motivated us to extend the formalism to allow for a dynamical mixing of states that are projected from low-lying (multi) particle-(multi)hole self-consistent MF configurations. In the context of the $\alpha_C$ calculations, the idea is to mix $0^+$ states projected from $|\varphi_Y\rangle$, $|\varphi_\pi\rangle$, and $|\varphi_2\rangle$ configurations, respectively. In such an approach, the $I = 0$ wave functions in an odd–odd $N = Z$ nuclei are approximated by:

$$|n; I = 0, T_z = 0\rangle = \sum_{i = X, Y, ZT \geq 0} \sum_{l \geq 0} \sum_{l' \geq 0} I(n, J = 0, T_0 = 0) \tilde{P}_{u,0,0}^J \tilde{P}_{l=0}^J |\varphi_i\rangle,$$

(14)
where the coefficients $f_{ij}^{n, J = 0, T_z = 0}$ are obtained by solving the Hill–Wheeler–Griffin (HWG) equation, and $n$ enumerates the HWG eigenstates. The HWG equation has, typically, three linearly independent solutions which, instead of $n$, can be conveniently labeled by approximate isospin quantum number: $|I = 0, T \approx 0, T_z = 0\rangle$, $|I = 0, T \approx 1, T_z = 0\rangle$, and $|I = 0, T \approx 2, T_z = 0\rangle$.

The new set of the ISB corrections calculated using this prescription is displayed in figure 10; the detailed values can be found in [60]. The improved corrections are somewhat smaller that the values of [30] obtained by averaging over orientations. This difference, however, has almost no influence on $\mathcal{F}_T$ and $|V_{cd}|$. Indeed the new values $\mathcal{F}_T = 3073.7(11)$s and $|V_{ud}| = 0.97396(25)$, calculated with the updated set of experimental $f_t$ values taken from [45], almost perfectly match the previous numbers [30].

Towner and Hardy [43] proposed a confidence level test to check a consistency of the calculated ISB corrections. The underlying assumptions are: (i) validity of the CVC hypothesis up to at least $\pm 0.03\%$ and (ii) validity of the calculated nuclear-structure-dependent corrections $\delta_{NS}$ [41]. These two assumptions allow to calculate empirical corrections:

$$\delta_c^{(\exp)} = 1 + \delta_{NS} - \frac{\mathcal{F}_T}{f_t(1 + \delta_q^2)}.$$  \hspace{1cm} (15)

By treating the value of $\mathcal{F}_T$ as an adjustable parameter, one can bring $\delta_c^{(\exp)}$ as close as possible to the calculated $\delta_c$ by minimizing the appropriate $\chi^2$. With the new set of corrections calculated in [60], the $\chi^2$ per degree of freedom ($n_d = 11$) drops from $\chi^2 / n_d = 10.2$ [30] to 6.3. This number is still much larger than the values reported in [43], which are: 1.7 for the Damgård model [52], 0.4 for the shell-model with Woods–Saxon wave functions [45], 2.3 for the shell-model with Hartree–Fock wave functions [45], and 2.1 for the relativistic DFT+RPA model of [55]. The main contribution to the $\chi^2$-value in our model can be associated with the sudden increase in $\delta_c$ due to a single $^{62}$Ga $\rightarrow ^{62}$Zn transition, which contributes more than 62% to the total $\chi^2$ budget.

4. G.s. beta-transitions in $T = 1/2$ mirror nuclei

The $T = 1/2$ mirror nuclei offer an alternative way to test the CVC hypothesis [63]. These nuclei decay via the mixed Fermi and GT transitions. Hence, apart from the radiative and the ISB corrections, the values of $G_F$ and $V_{ud}$ also depend on the ratio of statistical rate functions $f_{SA}/f_{SV}$ for the axial-vector and vector interactions, and the ratio $\rho \approx \lambda M_{GT}/M_F$ of nuclear matrix elements, where $\lambda = g_A/g_V$ denotes the ratio of axial-vector and vector coupling constants.

The CVC hypothesis implies that the vector coupling constant is $g_V = 1$. The axial-vector current is partially conserved; this implies that the axial-vector coupling constant gets renormalized in the nuclear medium. The effective axial-vector coupling constant, $g_A^{(eff)} = g_V g_A$, is quenched by an $A$-dependent factor $q_A$ with respect to the free neutron decay value $g_A \approx 1 - 1.2701(25)$. Quenching factors deduced from comparison of large-scale NSM calculations with experiment are: $q_5 \approx 0.82$, 0.77 [64], and 0.74 [65] in the p-, sd-, and pf-shell region, respectively. In the region $A \approx 130$, a large value of $q_5 \approx 0.57$ has been extracted [66], see however [67]. To account for the mass dependence of $q_A$ in shell-model calculations, a phenomenological expression

$$q_A = 1 - 0.19 \left( \frac{A}{16} \right)^{0.35}$$  \hspace{1cm} (16)

has been proposed [64] for $A \leq 40$.

The origin of the quenching is not fully understood. It is usually related to missing correlations in the wave function; truncation of model space; and—in the context of ab initio models—two-body currents [68–70]. Much work in this area has been done in relation to the double-beta decay [70–72] and WIMP scattering [73]. Recent studies of the Ikeda sum rule in $\beta$ decays of $^{14}$C and $^{22,24}$O performed in [74] estimate quenching due to the two-body currents to be $q_5 = 0.84 - 0.92$. This range is consistent with experimental data on $^{96}$Zr [75, 76].

Recently, a systematic study of both the GT and Fermi g.s. transitions in the $T = 1/2$ mirror sd- and pf-shell nuclei $T = 1/2$ mirror nuclei with $17 \leq A \leq 55$ have been carried out using the self-consistent NCCI approach [77]. Within the NCCI model the wave function reads (see equation (6)):

$$\langle n; IM; T_z \rangle = \sum_{ij} a_{ij}^{(n, IM; T_z)} \langle \varphi_i^j; IM; T_z \rangle,$$

and

$$a_{ij}^{(n, IM; T_z)} = \sum_{ij} \sum_{K, T, T'} f_{ij}^{(n, IM; T_z)} P_{T, T'}^{MT} \tilde{P}_{MT}^{(n, IM; T_z)}.$$  \hspace{1cm} (17)

When compared to the isospin- and angular-momentum MR-DFT wave-function (6), the NCCI wave function contains additional summation over the configurations (Slater determinants) $\langle \varphi_i^j \rangle$. In the present implementation of the formalism,
we use the same Skyrme interaction to compute the configurations |φj⟩ and to mix the isospin- and angular-momentum-projected states |φj; IM; Tz⟩\(^{01}\).

The model was tested for the \(^6\text{He} \rightarrow ^6\text{Li}\) GT beta decay. Matrix element for this transition, |M_{GT}| = 2.1645(43), is precisely known from the recent measurement\(^{78}\), Figure 11 shows a difference between the calculated and experimental GT matrix element as a function of the NCCI configuration space considered. The first point corresponds to the case of no configuration mixing. Here, the wave functions |0^1_{pg}\rangle and |1^1_{pg}\rangle are projected from the optimal (energy-wise) Slater determinants. Next, keeping the parent wave function |0^1_{pg}\rangle fixed, we enrich the configuration space of the daughter nucleus by admixing the 1^+ states projected from the lowest particle–hole (ph) and the two lowest (2ph) particle–hole configurations: |1^1_{pg}\rangle → |1^1_{2ph}\rangle → |1^1_{3ph}\rangle. This causes an increase of the matrix element circa 3% above the experimental value. The extension of the configuration space of \(^6\text{He}\) by admixing excited 0^+ states hardly impacts this result, see figure 11. This test indicates that NCCI is capable of capturing the main features of the wave functions that are important for a reliable reproduction of the GT matrix element. Unfortunately, the model underbinds \(^6\text{Li}\) and overbinds \(^6\text{He}\); hence we have not great confidence in its accuracy for this specific GT transition. This is, however, not surprising as the current DFT approaches and their MR-DFT and NCCI extensions have not been optimized to experimental data in light nuclei.

Theoretical g.s. GT matrix elements in the \(T = 1/2\) mirror sd- and pf-shell nuclei ranging from \(A = 17\) till \(55\) are shown in figure 12. The NCCI results with the SV_{SO} EDF were obtained using the HFODD solver\(^{28, 79}\) that has been augmented with the NCCI module. The details of calculations follow\(^{77}\). It is seen that the NCCI results are fairly close to shell model predictions\(^{65, 80, 81}\). The consistency between these two theoretical approaches is visualized in figure 12(b), which shows that both models correlate well with experimental data. As discussed in\(^{77}\), this similarity is quite surprising since the models differ in many aspects.

The model-independent Ikeda sum rule\(^{82}\) serves as an important indicator of the quality of theoretical models of GT decay. In the \(A = 39, T_z = \pm 1/2\) nuclei, which can be viewed as one-hole systems, inclusion of all possible ph excitations within the sd-shell space exhausts 99% of the sum rule\(^{77}\). Recently, we have performed similar calculations for the \(A = 23, T_z = \pm 1/2\) systems, which are complex, open-shell deformed nuclei. The calculations, involving eight deformed particle–hole configurations, were performed using two variants of the NCCI model: the full model involving the isospin- and angular-momentum projection and its simplified variant involving only the angular-momentum projection. The results are shown in figure 13. As anticipated, both methods give almost identical matrix elements for the GS transition. This is because the effect of isospin mixing in the g.s.s of nuclei considered is very small. Note however, that the variant involving the angular-momentum projection only captures mere 40% of the Ikeda sum rule. At the same time, the full variant of the model accounts for 75% of the sum rule. The example shows that the proper treatment of isospin in excited states is critical for the sum rule evaluation. In order to improve the description of the Ikeda sum rule within the simplified model, one would need to increase the model space by invoking particle–hole configurations obtained by exciting core nucleons from the initial Nilsson level originating from the \(d_3/2\) shell to the Nilsson levels originating from the \(s_1/2\) and \(d_3/2\) shells. Such systematic calculations are in progress and will be published elsewhere.

The full variant of the model involving double-projection is necessary to compute the ISB corrections to the Fermi branch of beta-decay in the \(T = 1/2\) mirror nuclei. These nuclei offer independent way to verify the CVC hypothesis.
and to study the CKM matrix\textsuperscript{[63, 84]}. A set of the ISB corrections calculated with the MR-DFT technique was published in\textsuperscript{[57]}, and the NCCI results can be found in table 1 of\textsuperscript{[77]}. The NCCI predictions are shown in figure 14 and compared to the SM results of\textsuperscript{[83]}. It is seen that the NCCI corrections, although slightly smaller on average, are fairly consistent with SM. Figure 15 shows a difference between these two sets of calculations. The shaded area marks the error band calculated as $\sqrt{(\Delta \delta_C^{\text{NCCI}})^2 + (\Delta \delta_C^{\text{SM}})^2}$ under the assumption of 10% error on the NCCI results due to a basis cut-off.

5. Mirror and triplet binding energy differences, and the Nolen–Schiffer anomaly

Strong interaction is, predominantly, invariant with respect to rotations in the isospin space. This fact is rather well established experimentally and confirmed theoretically. Indeed, most nuclear many-body approaches, including shell-model and DFT models, use interactions that are scalar in the isospin space. The Skyrme interaction is a prime example of an isospin invariant effective force that has long been used to compute various nuclear properties.

On the other hand, there also exists a firm experimental evidence that the strong interaction contains small isospin-breaking components. For example, the nucleon–nucleon (NN) scattering data reveal small differences in phase shifts and scattering lengths. In the $^1S_0$ channel, the scattering lengths for neutron–neutron (nn), np, and proton–proton (pp) scattering are: $a_{nn} \approx -18.9$ fm, $a_{np} \approx -23.7$ fm, and $a_{pp} \approx -17.3$ fm, respectively\textsuperscript{[85]}. A detailed analysis of scattering data, in particular phase shifts and scattering lengths, shows that the nn interaction is 1% stronger than pp interaction and that the np interaction is 2.5% stronger than the average of nn and pp interactions\textsuperscript{[85]}. (These figures include corrections for electromagnetic effects and refer solely to the strong NN interaction.) On the fundamental level, the isospin symmetry is broken due to different masses and electromagnetic interactions of $u$ and $d$ quarks\textsuperscript{[86]}. Albeit small, isospin violation considerably influences global properties of finite nuclei such as binding energies. It is well known that models including isospin-invariant strong force and the Coulomb interaction alone have difficulties in reproducing the mirror displacement energies (MDEs), the differences of binding energies of mirror nuclei (Nolen–Schiffer anomaly\textsuperscript{[87]}):

$$\text{MDE} = BE(T, T_z = -T) - BE(T, T_z = +T).$$

These models have also problems in reproducing the triplet displacement energies (TDEs). The TED indicator is defined...
as:

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

(19)

and is a measure of the binding-energy curvature within the isospin triplet [36, 88–90].

It is customary to classify components of the nuclear force in terms of the SU(2) symmetry of isospin. Here, one defines charge independence as invariance under rotation in the isospin space. The charge symmetry, on the other hand, can be defined as an invariance under a rotation by 180° about the y isospin axis. Violation of this symmetry is referred to as charge symmetry breaking (CSB).

In the language of NN force, CSB implies a difference between pp and nn interactions in the same channel, \( V_{\text{CSB}} \neq V_{\text{pp}} \). Moreover, if in the isospin-triplet \( T = 1 \) channel \( V_{\text{CSB}} = (V_{\alpha \alpha} + V_{\beta \beta})/2 \) the force is charge-independence-breaking (CIB). The data on NN scattering lengths indicate that the presence of isospin-conserving nuclear forces. If neglected, or not treated carefully, the continuum effects can alter results of such analyses [106–108].

The ISB components of NN interactions were studied in \textit{ab initio} approaches [85, 93]. Hadronic ISB terms of effective NN interactions were investigated in the context of NSM [88, 94–100] and MF approaches [54, 101–103]. A note of caution is in order here. First, any attempt to extract effective NN interactions from spectroscopic data should first account for the coupling to the many-body continuum [104, 105] in the presence of isospin-conserving nuclear forces. If neglected, or not treated carefully, the continuum effects can alter results of such analyses [106–108]. Second, in-medium nuclear effective interactions (G-matrix) contain contributions from the Coulomb force. If the Coulombic contributions are not treated precisely during the renormalization procedure, they can result in the presence of CSB and CIB components, which can then be incorrectly labelled as ‘hadronic’.

To investigate the effect of hadronic CSB and CIB terms and their possible influence on isospin mixing and ISB corrections, one can apply the local Skyrme-DFT approach. To this end, one needs to generalize the formalism to the case of pn-mixed quasiparticle states [109]. Such an extension leads to isospin-invariant EDFs that depend explicitly on local pn densities and currents. Recently, this formalism was applied to the Hartree–Fock case by admitting pn mixing in the particle–hole channel [110, 111]. Within this framework, the explicit ISB comes entirely from the electrostatic interaction.

In the next step, the pn-mixed formalism can be extended to accommodate the CSB and CIB hadronic components. The pn-mixing is a necessary prerequisite that allows to study these terms in a fully self-consistent manner. Since the discrepancies between the experimental and theoretical MDEs and TDEs are small [36, 103] they can be modelled in terms of class II (CIB) and class III (CSB) zero-range corrections to the conventional Skyrme force:

\[
\hat{V}_{\text{II}}(i,j) = \frac{1}{2} t_{0}^{\text{II}} \delta(\rho_{i}) (\rho_{i} - \rho_{j}) (\rho_{j} - \rho_{i} \sigma_{i} \sigma_{j}),
\]

\[
\hat{V}_{\text{III}}(i,j) = \frac{1}{2} t_{0}^{\text{III}} \delta(\rho_{i}) (\rho_{i} + \rho_{j}),
\]

where \( t_{0}^{\text{II}} \) and \( t_{0}^{\text{III}} \) are the ISB force parameters that are adjusted to reproduce empirical TDEs and MDEs. The spin-exchange has been omitted as it leads to a trivial rescaling of the parameters. The associated ISB contributions to the EDF are:

\[
\mathcal{H}_{\text{II}} = \frac{1}{2} t_{0}^{\text{II}} \rho_{i}^{2} - 2 \rho_{i} \rho_{j} \rho_{j} \rho_{i} - 2 \rho_{i}^{2} \rho_{j}^{2} - 2 s_{j}^{2},
\]

\[
\mathcal{H}_{\text{III}} = \frac{1}{2} t_{0}^{\text{III}} \rho_{i}^{2} - 2 \rho_{i}^{2} - 2 s_{j}^{2} + 2 s_{i}^{2} + 2 s_{j}^{2} + 2 s_{i}^{2} + 2 s_{j}^{2}.
\]

Note, that class II forces depend on the pn-mixed particle \( \rho_{\text{op}} \) and spin \( s_{\text{op}} \) densities, respectively. Hence, these forces can be included only within the pn-mixed DFT formalism. The class III forces, on the other hand, depend only on the standard pp and nn densities and can be, therefore, treated within the conventional Skyrme-DFT approach.

In order to control the total isospin of the nucleus in the pn-mixing calculations, we use a three-dimensional isocranking approach [112]. This technique is analogous to the well known cranking method in real space, which is commonly used in high-spin physics. It is realized by adding the isocranking term to the MF Hamiltonian \( \hat{h} \):

\[
\hat{h} = \hat{h} - \hat{\Lambda} \hat{\sigma} i = \hat{h} - \lambda_{1} \hat{h}_{1} - \lambda_{2} \hat{h}_{2} - \lambda_{3} \hat{h}_{3},
\]

where \( \hat{\sigma} i = \frac{1}{2} \hat{\sigma} \) stands the s.p. isospin operator and \( \hat{\Lambda} \) is the isocranking frequency. By adjusting the frequencies \( \lambda \), one can control both the length and direction of the isospin vector.
In practical applications, $\lambda$ is parameterized as follows:

$$\lambda = (\lambda' \sin \theta' \cos \phi, \lambda' \sin \theta' \sin \phi, \lambda' \cos \theta' + \lambda_{\text{off}}).$$  \hspace{1cm} (25)

The offset $\lambda_{\text{off}} \neq 0$ is introduced to facilitate calculations with the Coulomb interaction [110, 111]. By choosing the offset properly, one can compensate for the effect of the electrostatic interaction on the third component of the isocranking term. In this way, $\lambda_{\text{off}}$ helps to avoid s.p. level crossings while tilting the isocranking axis and, consequently, keeps the expectation value of the total isospin fixed [113].

In order to study the influence of the ISB forces on nuclear binding energies, we have performed the isocranking calculations for the $A = 34$ isospin triplet. In these test calculations, the Coulomb interaction has been switched off. The results with the CIB force (20) are shown in figure 16.

As anticipated, this force impacts the binding energy of $T_z = 0$ system without affecting the binding energies of $T_z = \pm 1$ triplet members. Hence, it changes the TDE indicator without affecting MDE. On the other hand, as shown in figure 17, the class III force (21) changes MDEs without affecting TDEs. This implies that the simplest strategy is to adjust the coupling constants $t_{0}^{II}$ and $t_{0}^{III}$ to TDEs and MDEs, respectively.

Figure 18 and 19 show preliminary results of the calculated MDEs and TDEs in the isospin triplets ranging from $A = 22$ to 55. The calculations have been done using the SV Skyrme EDF with Coulomb, augmented by the CIB and CSB forces with $t_{0}^{II} = 20$ MeV and $t_{0}^{III} = -8$ MeV, respectively. It is seen that a generalized pn-mixed Skyrme DFT approach is able to reproduce experimental data on TEDs and MDEs.

The pn-mixed ISB DFT formalism can address the evolution of ISB effects with angular momentum in rotational bands of $T = \frac{1}{2}$ and $T = 1$ nuclei. Such effects have been investigated within shell-model framework [88, 95, 96, 98, 99, 114, 115]. The quantities of interest are mirror energy differences (MDEs) and triplet energy differences (TEDs), similar to MDEs and TDEs but defined through excitation energies $\Delta E_I$ of rotational states at a given angular momentum $I$:

$$\text{MED}(I) = \Delta E_I \left(T = \frac{1}{2}, T_z = -\frac{1}{2}\right) - \Delta E_I \left(T = \frac{1}{2}, T_z = +\frac{1}{2}\right).$$  \hspace{1cm} (26)
reproduce rotational bands. The preliminary calculations with Skyrme forces with low effective mass is its ability to especially in the upper fp shell. MEDs and TEDs, the overall picture is not fully understood, for the explanation of angular momentum dependence of hadronic forces are as important as the Coulomb interaction. In general, while shell-model studies indicate that the ISB behind the pair condensate works irrespective of details of the underlying interaction that couples fermions into the Cooper pairs at the Fermi surface. In low-energy nuclear physics, nucleonic pairing affects many properties of finite nuclei and nucleonic matter [118, 119].

Nucleonic Cooper pairs can exist in many flavors. In terms of isospin quantum number, one can talk about isovector triplet \((T = 1)\) and isovector singlet \((T = 0)\) pairs. The conventional \(nn\) and \(pp\) pairing has isovector character, while the \(pn\) pairing can be either isovector or isoscalar. The first attempts to incorporate the \(pn\)-pairing into the independent quasi-particle approach date back to the mid-sixties [120–122]. These models were further developed into a consistent formalism allowing for simultaneous treatment of isovector and isoscalar pairs [123–128]. The formalism was further extended to include stretched \(T = 0\) pairs (\(aa\) \(pn\)-pairing) in [129]. These early approaches encountered difficulties in predicting coexisting \(T = 0\) and \(T = 1\) pairing-phases. The solutions of the early models based on separable seniority-type interactions could be conveniently classified in terms of a single parameter, the value of isoscalar-to-ivector matrix element ratio \(x \equiv G(T=0)/G(T=1)\). In particular, for \(N = Z\) nuclei, the solution is of a pure isovector type for \(x < 1\); for \(x = 1\) the isovector and isoscalar phases are degenerate; and for \(x > 1\) there appears a pure isoscalar solution. These models were later extended [130] to include particle-number projected wave functions. For \(x > x_{\text{crit}} \approx 1.1\), the extended models have produced coexistence of \(T = 0\) and \(T = 1\) phases. It was also predicted that for \(x \geq 1.3\) the isoscalar pairing component could be the source of the Wigner energy [8, 130]. Following these developments, various models have been proposed to look for signatures of the isoscalar pairing phase and explain the Wigner energy [9, 131–139].

In spite of many efforts, however, a comprehensive theory of nucleonic pairing still eludes us. This negatively impacts our understanding of nuclei in the vicinity of the \(N = Z\) line, where the \(pn\)-correlations are expected to be strongest. Indeed, a consistent approach to the \(pn\)-pairing problem requires implementing the \(pn\)-mixing on the MF level, whereby the s.p. wave functions are combinations of proton and neutron components. Basic self-consistency principles require such a mixing to accompany any hypothetical \(pn\)-mixing in the pairing channel. Moreover, the stability and existence of the \(pn\)-pairing condensate may critically depend on the restoring force related to the \(pn\)-mixing on the MF level, and thus both must be simultaneously included in the theoretical description. As discussed above, the DFT frameworks incorporating the \(pn\)-mixing have been developed recently [110, 111]. This constitutes the first step towards building a consistent symmetry-unrestricted superfluid DFT approach with the complete \(pn\)-mixing. The experience gathered so far indicates that in order to capture structure of \(N \approx Z\) nuclei, the \(pn\)-mixed formalism should be further extended to include the restoration of number symmetry and proper treatment of isospin [24, 113].

A need for the enhancement of the deuteron-like \(J = 1^+\), \(T = 0\) pairing channel is apparent in the present Skyrme-NCCI approach, which accounts relatively well for low-spin states but has systematic problems with the \(J = 1^+, T = 0\) matrix elements in \(N = Z\) nuclei. This is illustrated in

\[
\begin{align*}
\text{TED}(I) &= \Delta E_f(T = 1, I_z = -1) \\
&\quad - 2\Delta E_f(T = 1, I_z = 0) \\
&\quad + \Delta E(T = 1, I_z = +1).
\end{align*}
\]

In general, while shell-model studies indicate that the ISB hadronic forces are as important as the Coulomb interaction for the explanation of angular momentum dependence of MEDs and TEDs, the overall picture is not fully understood, especially in the upper fp shell.

One of the key features of the NCCI model based on Skyrme forces with low effective mass is its ability to reproduce rotational bands. The preliminary calculations performed for \(^{48}\text{Cr}\), a key nucleus in the f-shell concerning collective properties, indicate that our model is capable of reproducing its collective g.s. band fairly well [116]. This opens an opportunity to address MED and TED effects in a non-perturbative way, as a function of angular momentum, incorporating the ISB effects self-consistently along the rotational path.

6. Proton–neutron pairing

Superfluidity and superconductivity belong to the most spectacular examples of emergent phenomena in many-body systems. They appear at different physical scales and in different environments in atomic, condensed matter, nuclear, and elementary particle physics. The BCS mechanism [117] behind the pair condensate works irrespective of details of the underlying interaction that couples fermions into the Cooper...
The future developments will undoubtedly utilize the newly developed isospin-invariant density functional framework [110, 111]. The pn-mixed DFT formalism needs to be extended to the particle–particle channel by including pairing interaction of both isoscalar and isovector types. This will enable us to study the importance of the isoscalar pairing densities and fields on the structure of $N \approx Z$ nuclei and the impact of pn-mixing on single- and double-beta decays. It seems, however, that in order to capture key structural aspects of $N = Z$ nuclei, the pn-mixed formalism should be further extended to include the restoration of particle number, isospin, and angular momentum. This will require an appropriate NCCI extension.

In quantitative calculations, quality input is crucial. A construction and optimization of a realistic Hamiltonian-based EDF is among the most urgent needs. This development will not only improve the predictive power of the model but will also help addressing the burning question pertaining to the role of ISB interaction components.

Acknowledgments

Useful discussions with Jacek Dobaczewski are gratefully acknowledged. Paweł Bączyk is thanked for providing material presented in section 5 prior to publication [116]. This article is based upon work supported by the Polish National Science Centre (NCN) under Contract No. 2012/07/B/ST2/03907 and by the US Department of Energy, Office of Science, Office of Nuclear Physics under Award Numbers No. DOE-DE-SC0013365 (Michigan State University) and No. DE-SC0008511 (NUCLEI SciDAC Collaboration). The CSC-IT Center for Science Ltd, Finland, is acknowledged for the allocation of computational resources.

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