# Microscopic Calculations of Isospin-Breaking Corrections to Superallowed Beta Decay

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# Microscopic calculations of isospin-breaking corrections to superallowed $\beta$-decay

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The superallowed $\beta$-decay rates that provide stringent constraints on physics beyond the Standard Model of particle physics are affected by nuclear structure effects through isospin-breaking corrections. The self-consistent isospin- and angular-momentum-projected nuclear density functional theory is used for the first time to compute those corrections for a number of Fermi transitions in nuclei from $A = 10$ to $A = 74$. The resulting leading element of the CKM matrix, $|V_{\rm ud}| = 0.97447(23)$, agrees well with the recent result of Towner and Hardy [Phys. Rev. C **77**, 025501 (2008)].

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Nuclear $\beta$ decays provide us with the crucial information about the electroweak force and constraints on physics beyond the Standard Model [1, 2]. Of particular importance are superallowed Fermi transitions between the $J^\pi = 0^+$ members of an isospin multiplet that can be used to test the conserved vector current (CVC) hypothesis and provide the most restrictive test of the unitarity of the Cabibbo-Kobayashi-Maskawa (CKM) matrix. Under assumptions of zero energy transfer and pure isospin, the transition matrix elements for superallowed $\beta$ decays do not depend on nuclear structure.

For actual nuclei, however, small corrections to the Fermi matrix element of $J = 0^+, T = 1 \to J = 0^+, T = 1$ superallowed transitions must be applied (see Refs. [3–6] and Refs. quoted therein):

$$|M_F^{(\pm)}|^2 = 2(1 + \delta'_{\rm R})(1 + \delta_{NS} - \delta_C), \qquad (1)$$

where $\delta_C$ is a nuclear-structure-dependent isospin-breaking correction, and $\delta'_{\rm R}$ and $\delta_{NS}$ are radiative corrections. The corrected product of statistical rate function $f$ and partial half-life $t$ can be written as

$$ft = \frac{\mathcal{F}t}{(1 + \delta'_{\rm R})(1 + \delta_{NS} - \delta_C)} \qquad (2)$$

with $\mathcal{F}t$ being nucleus independent.

In spite of theoretical uncertainties in evaluation of radiative and isospin-breaking corrections, the superallowed $\beta$-decays provide a stringent test of the CVC hypothesis. In turn, it is also the most precise source of information on the leading element $V_{\rm ud}$ of the CKM matrix [5, 7]. Indeed, with the CVC hypothesis confirmed, $V_{\rm ud}$ can be extracted from the data by averaging over 13 precisely measured superallowed $\beta$ transitions spreading over a broad range of nuclei from $A = 10$ to $A = 74$ [5].

The main focus of this work is isospin-breaking corrections $\delta_C$. This topic has been a subject of numerous theoretical studies using different techniques [5, 8–13]. The standard in this field has been set by Hardy and Towner (HT) [4, 5, 14] who employed the nuclear shell model (SM) to account for configuration mixing and the mean-field approach to describe the radial mismatch of proton and neutron single-particle (s.p.) wave functions. Our approach to $\delta_C$ is based on the self-consistent isospin- and angular-momentum projected nuclear density functional theory (DFT) [15, 16]. This framework can simultaneously describe various effects that profoundly impact matrix elements of the Fermi decay; namely, symmetry breaking, configuration mixing, and long-range Coulomb polarization. It should also be noted that our method is quantum-mechanically consistent (see discussion in Ref. [12]) and contains no adjustable free parameters.

The isospin- and angular-momentum projected DFT approach is based on self-consistent states $|\varphi\rangle$ which, in general, violate both rotational and isospin symmetries. While the rotational invariance is broken spontaneously [17, 18], the isospin symmetry is broken both spontaneously (on DFT level) and directly by the Coulomb force. Consequently, the theoretical strategy is to restore the rotational invariance, remove the spurious isospin mixing present in the DFT wave function, and retain only the physical isospin mixing caused by the Coulomb interaction. This is achieved by the rediagonalization of the entire Hamiltonian, consisting the isospin-invariant kinetic energy and nuclear interaction (Skyrme) terms, and isospin-breaking Coulomb force, in a good-angular-momentum and good-isospin basis

$$|\varphi; IMK; TT_z\rangle = \mathcal{N}\hat{P}^T_{T_zT_z}\hat{P}^I_{MK}|\varphi\rangle, \qquad (3)$$

where $\hat{P}^T_{T_zT_z}$ and $\hat{P}^I_{MK}$ stand for the isospin and angular-momentum projection operators and $\mathcal{N}$ is the normalization factor. In the current version of the model, nuclear isospin-breaking interactions and pairing have been disregarded.

The set of states (3) is, in general, overcomplete be-

cause the $K$ quantum number is not conserved. This difficulty is overcome by selecting first the subset of linearly independent states (collective space), which is spanned, for each $I$ and $T$, by the natural states $|\varphi;\, IM;\, TT_z\rangle^{(i)}$ that are eigenstates of the overlap matrix [19, 20]. Diagonalization of the Hamiltonian in the collective space yields the eigenfunctions:

$$|n;\, \varphi;\, IM;\, T_z\rangle = \sum_{i,T\geq|T_z|} a_{iIT}^{(n;\varphi)} |\varphi;\, IM; TT_z\rangle^{(i)}, \quad (4)$$

where the index $n$ labels eigenstates in ascending order according to their energies while $I$, $M$, and $T_z = (N-Z)/2$ are strictly conserved. By construction, vectors (4) are free from spurious isospin mixing. Moreover, since projection is applied to self-consistent DFT solution, a subtle interplay between the Coulomb polarization (that tends to make the proton and neutron wave functions different) and the short-range nuclear attraction (acting in exactly the opposite way) is properly taken into account. As discussed in Refs. [15, 16, 21, 22], direct inclusion of monopole polarization effect, which is crucial for evaluation of isospin mixing in open-shell heavy nuclei, excludes all core-based models thus leaving us with essentially one choice: the nuclear DFT. Recent experimental data on isospin impurities deduced in $^{80}$Zr from the giant dipole resonance $\gamma$-decay studies [23] are consistent with the magnitude of isospin mixing calculated with isospin-projected DFT [22], and this is very encouraging.

As demonstrated in Ref. [21], in odd-odd $N = Z$ nuclei, the isospin projection alone is not sufficient and a simultaneous angular-momentum projection is a must. Unfortunately, this leads to the appearance of singularities in the energy kernels [22], thus preventing us from using modern Skyrme energy density functionals (EDFs) as none of them is usable, whereas those depending on integer powers of the density, which are regularizable [24], are not yet developed. Hence, at present, the only practical option is to use the Hamiltonian-driven EDFs which, for Skyrme-type functionals, leaves only one option: the density-independent SV parametrization [25] supplemented by tensor terms.

The unusual form of SV impacts negatively its overall spectroscopic quality by impairing such key properties as the symmetry energy [22], level density, and level ordering. These deficiencies affect the calculated isospin mixing. For instance, for the case of $^{80}$Zr discussed above, SV yields the isospin mixing 2.8%, i.e., smaller than the mean isospin mixing 4.4% averaged over nine commonly used Skyrme EDFs, see Fig. 1 of Ref. [21]. Of course, for the description of $\delta_C$, of importance is not the absolute magnitude of isospin mixing but its difference between parent and daughter states [13]. The lack of reasonable EDF is, admittedly, the weakest point of our current calculations; nevertheless, no significant improvement of this aspect can be expected in the near future.

The $0^+ \to 0^+$ Fermi $\beta$-decay proceeds between the $|I = 0, T \approx 1, T_z = \pm 1\rangle$ ground state (g.s.) 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. While the DFT state representing the even-even nucleus is unambiguously defined, the DFT state used to compute the $N = Z$ wave function is the so-called anti-aligned configuration $|\varphi\rangle \equiv |\bar{\nu} \otimes \pi\rangle$ (or $|\nu \otimes \bar{\pi}\rangle$), selected by placing the odd neutron and the odd proton in the lowest available time-reversed (or signature-reversed) s.p. orbits. The anti-aligned configurations manifestly break the isospin symmetry but they provide a way to reach the $|T \approx 1, I = 0\rangle$ states in odd-odd $N = Z$ nuclei [16]. This situation creates additional technical problems. The anti-aligned configurations appear to be very difficult to converge in the symmetry-unrestricted DFT calculations. This can be traced back to time-odd components of the EDF. In fact, only in a few cases were we able to obtain symmetry-unrestricted self-consistent solutions. This forced us to impose the signature-symmetry on other DFT wave functions, which implied a specific s.p. angular-momentum alignment pattern [26].

The calculations presented here were done using the DFT solver HFODD (v2.48q) [19], which includes both the angular-momentum and isospin projection. The calculated values of $\delta_C$ depend on the basis size. In order to obtain converged result for $\delta_C$ with respect to basis truncation, we use 10 oscillator shells for $A < 40$ nuclei, 12 oscillator shells for $40 \leq A < 62$ nuclei, and 14 oscillator shells for $A \geq 62$ nuclei. The resulting systematic errors due the basis cut-off do not exceed $\sim$10%.

The equilibrium quadrupole deformations $(\beta_2, \gamma)$ of the anti-aligned configurations in odd-odd nuclei are, in most cases, very close to those obtained for even-even isobaric analogs. Typical differences do not exceed $\Delta\beta_2 \approx 0.005$ and $\Delta\gamma \approx 1^\circ$ except for nearly spherical systems $A = 14$ and $A = 42$, where the concept of static deformation is ill-defined, and for $A = 10$ and $A = 18$ pairs where odd-odd and even-even partners have fairly different shapes. As we shall see below, such deformation difference results in large values of $\delta_C$.

All studied odd-odd nuclei, except for $A = 14$, 38, and 42, are deformed; thus, to carry out projections, we could use for them the unique lowest anti-aligned DFT states. Also for $A = 14$ and 38, unique configurations based on the $1p_{1/2}$ and $2s_{1/2}$ subshells were used. A different approach was used to compute $\delta_C$ in near-spherical $A = 42$ nuclei. In $^{42}$Sc, four possible anti-aligned DFT configurations built on the s.p. orbits originating from the spherical $1f_{7/2}$ subshells can be formed, and the corresponding DFT states differ slightly due to configuration-dependent polarizations [21]. Consequently, to evaluate $\delta_C$ for $A = 42$ we took an arithmetic mean over the values calculated for all anti-aligned configurations.

The unusually large correction $\delta_C \approx 10\%$ has been calculated for $A = 38$ nuclei. Most likely, this is a con-

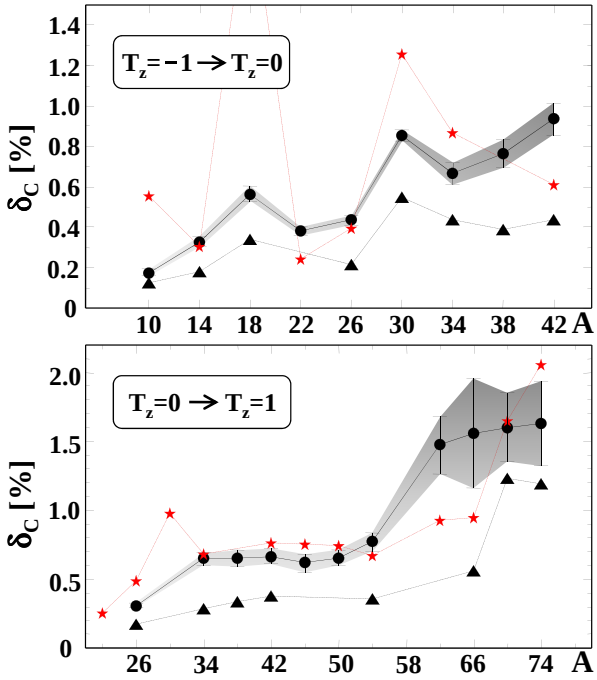


FIG. 1: (Color online) Calculated isospin-mixing corrections $\delta_C$ for $T_z = -1 \rightarrow T_z = 0$ (top) and $T_z = 0 \rightarrow T_z = 1$ (bottom). Our adopted values (stars) are compared to values of Ref. [5] (dots; including errors) and Ref. [11] (triangles).

sequence of incorrect shell structure predicted with SV. Specifically, as a result of incorrect balance between the spin-orbit and tensor terms in SV, the $2s_{1/2}$ subshell is shifted up to the Fermi surface. This state is more sensitive to time-odd polarizations than other s.p. states around $^{40}$Ca core, see Table I in Ref. [27]. Consequently, the $^{38}$K$\rightarrow^{38}$Ar transition has been excluded from our calculation of $V_{\rm ud}$.

The adopted values of $\delta_C$ are shown in Fig. 1 for the $T_z = -1 \rightarrow T_z = 0$ transitions in light systems (upper panel) and for $T_z = 0 \rightarrow T_z = 1$ transitions pertaining to heavier systems (lower panel). It is instructive to compare our results to those of Refs. [5] and [11]. In light nuclei, the calculated $\delta_C$ are sensitive to the local shell structure. Indeed, although our values of $\delta_C$ show roughly the same trend as those of Ref. [5], the individual values differ. The reason can be traced back to the poor spectroscopic quality of SV, which manifests itself much stronger in light than in heavier nuclei due to the low s.p. level density. Let us also remind that the equilibrium minima in parent and daughter nuclei with $A = 10$ and $A = 18$ differ, and this results in increased $\delta_C$ values. As verified by DFT calculations using other EDFs, and also findings of Ref. [11], with higher level density in heavier nuclei the detailed shell structure seems to play a lesser role. This indicates that gross features of configuration mixing in heavier nuclei associated with long-range time-even (shape) correlations are less dependent on a EDF

TABLE I: Experimental $ft$-values (in sec); $\delta_C$ values adopted in this work (in %); calculated $\mathcal{F}t$-values (in sec); empirical corrections (5) (in %), and individual contributions to $\chi^2$ used in the CL test.

| Parent | $ft$ | $\delta_C$ | $\mathcal{F}t$ | $\delta_C^{(\rm EXP)}$ | $\chi^2_i$ |
|---|---|---|---|---|---|
| $T_z = -1$ : | | | | | |
| $^{10}$C | 3041.7(43) | 0.559(56) | 3064.8(48) | 0.39(14) | 1.3 |
| $^{14}$O | 3042.3(11) | 0.303(30) | 3072.3(21) | 0.38(06) | 1.5 |
| $^{22}$Mg | 3052.0(70) | 0.243(24) | 3082.2(71) | 0.64(23) | 3.0 |
| $^{34}$Ar | 3052.7(82) | 0.865(87) | 3063.5(87) | 0.65(27) | 0.6 |
| $T_z = 0$ : | | | | | |
| $^{26}$Al | 3036.9(09) | 0.494(49) | 3066.7(20) | 0.39(04) | 6.8 |
| $^{34}$Cl | 3049.4(11) | 0.679(68) | 3069.8(26) | 0.67(05) | 0.0 |
| $^{42}$Sc | 3047.6(12) | 0.767(77) | 3069.2(31) | 0.74(06) | 0.1 |
| $^{46}$V | 3049.5(08) | 0.759(76) | 3069.0(30) | 0.73(06) | 0.3 |
| $^{50}$Mn | 3048.4(07) | 0.740(74) | 3068.3(31) | 0.69(07) | 0.7 |
| $^{54}$Co | 3050.8(10) | 0.671(67) | 3073.0(32) | 0.77(08) | 1.5 |
| $^{62}$Ga | 3074.1(11) | 0.925(93) | 3088.7(41) | 1.52(09) | 41.0 |
| $^{74}$Rb | 3084.9(77) | 2.06(21) | 3064(11) | 1.88(27) | 0.4 |

parametrization and may be relatively well captured by SV. The calculated values of $\delta_C$ for heavier nuclei are indeed quite consistent with the HT results [5], with the exception of $A = 62$ and 66.

The predicted isospin-breaking corrections are listed in Table I. All other ingredients needed to compute $\mathcal{F}t$-values from Eq. (2), including empirical $ft$-values and radiative corrections $\delta'_{\rm R}$ and $\delta_{NS}$, were taken from the most recent compilation [28]. In the error budget of $\mathcal{F}t$ in Table I, apart from errors of $ft$ and radiative corrections, we include 10% systematic uncertainty in the calculated $\delta_C$ due to basis truncation. The average value $\overline{\mathcal{F}t} = 3070.4(9)$ s was obtained using Gaussian-distribution-weighted formula to conform with standards set by HT. This leads to $|V_{\rm ud}| = 0.97447(23)$ which coincides with both the HT result $|V_{\rm ud}^{(\rm HT)}| = 0.97418(26)$ [5] and a central value obtained from the neutron decay $|V_{\rm ud}^{(\nu)}| = 0.9746(19)$ [7]. Combining the calculated $|V_{\rm ud}|$ with the values of $|V_{\rm us}| = 0.2252(9)$ and $|V_{\rm ub}| = 0.00389(44)$ provided in Ref. [7], we obtain $|V_{\rm ud}|^2 + |V_{\rm us}|^2 + |V_{\rm ub}|^2 = 1.00031(61)$, which implies that unitarity of the CKM matrix is satisfied with precision of 0.1%.

While our value of $|V_{\rm ud}|$ is consistent with both HT and neutron-decay results, a question arises about its confidence level, especially in light of poor spectroscopic properties of SV. To this end, we carry out the confidence-level (CL) test proposed recently in Ref. [28] using variant including uncertainties on experiment, $\delta'_{\rm R}$, and $\delta_{NS}$. The test is based on the assumption that the CVC hypothesis is valid to at least $\pm 0.03\%$ precision, implying that a set of structure-dependent corrections should produce a statistically consistent set of $\mathcal{F}t$ values. Since only one set of

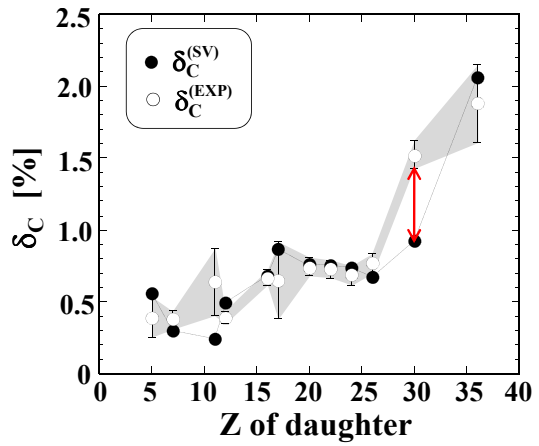


FIG. 2: (Color online) Calculated (black dots) and empirical (white dots, with error bars) values of $\delta_C$ as function of proton number in the daughter nuclei. Vertical arrow marks the values for $A = 62$. See text for details.

calculated $\delta_{NS}$ corrections exists [3], "empirical" isospin-symmetry-breaking corrections can thus be defined by

$$\delta_C^{(\mathrm{EXP})} = 1 + \delta_{NS} - \frac{\overline{\mathcal{F}t}}{ft(1+\delta'_{\mathrm{R}})}, \qquad (5)$$

and they are tabulated in Table I. The CL can be assessed by minimizing the root mean square deviation between predicted and empirical values of $\delta_C$ with respect to $\overline{\mathcal{F}t}$ in Eq. (5). The final result corresponding to $\overline{\mathcal{F}t} = 3070.0\,\mathrm{s}$ is shown in Fig. 2. Individual contributions to $\chi^2$ are also displayed in Table I. Our value of reduced $\chi^2$ (per degree of freedom; in our case $n_d = 11$) is 5.2. This is considerably higher than the values reported in Ref. [28] for the Damgaard model [8, 14] (1.7), SM with Woods-Saxon radial wave functions [5] (0.4), SM with Hartree-Fock (HF) radial wave functions [4, 9] (2.2), and relativistic Hartree plus RPA model of [11] (2.1). The low CL of our model results primarily from the single point at $A = 62$.

In summary, the state-of-the-art isospin- and angular-momentum-projected DFT calculations have been performed to compute the isospin-breaking corrections to $0^+ \to 0^+$ Fermi superallowed $\beta$-decays. Our results for $\bar{\mathcal{F}}t = 3070.4(9)\,\mathrm{s}$ and $|V_{\mathrm{ud}}| = 0.97447(23)$ were found to be consistent with the recent HT value [5]. While the CL of our $\delta_C$ values is low, primarily due to a poor spectroscopic quality of the EDF used, our framework contains no adjustable parameters and is capable of describing microscopically all elements of physics impacting $\delta_C$. The results presented in this paper should thus be considered as a microscopic benchmark relative to which the further improvements (e.g., regularizable EDF and/or inclusion of pairing) will be assessed.

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