Beta-decay study within multi-reference density functional theory and beyond

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Pioneering study of Gamow-Teller (GT) and Fermi matrix elements (MEs) using no-core-configuration-interaction formalism rooted in multi-reference density functional theory is presented. After successful test performed for $^4\text{He} \to ^4\text{Li}$ $\beta$-decay, the model is applied to compute MEs in the $sd$- and $pf$-shell $T=1/2$ mirror nuclei. The calculated GT MEs and the isospin-symmetry-breaking corrections to the Fermi branch are found to be in a very good agreement with shell-model predictions in spite of fundamental differences between these models concerning model space, treatment of correlations or inclusion of a core. This result indirectly supports the two-body current based scenarios behind the quenching of axial-vector coupling constant.

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The atomic nuclei are unique laboratories to study fundamental processes and search for possible signals of new physics beyond the Standard Model in ways that are complementary or even superior to other sciences. This is due to enhanced sensitivity of specific isotopes to fundamental symmetries caused, in particular, by intrinsic-symmetry-related or purely accidental (near-) degeneracies of nuclear states. For example, parity doublets caused by stable octupole deformation increase sensitivity to the violation of CP-symmetry which is responsible for matter over anti-matter dominance Universe [1]. Accidental near-degeneracy of $3/2^+$ is responsible for matter over anti-matter dominated Universes [2]. Last but not least, nuclear physics input is critical in an ongoing hunt for a weakly-interacting massive particle (WIMP), a candidate for dark matter, in direct detection experiments measuring the recoil energy deposited when WIMP is scattered off the nucleus, see [3] and refs. quoted therein.

Traditionally, the atomic nuclei are used to study the weak interaction. A flagship example is the superallowed $I=0^+ \to I=0^+ \beta$-decay among the members of the isobaric triplets $T=1$. With small, of order of a percent, theoretical corrections accounting for radiative processes and isospin symmetry breaking (ISB), these semileptonic pure Fermi (vector) decays allow to verify the conserving vector current (CVC) hypothesis with a very high precision. In turn, they provide the most precise values of the strength of the weak force, $G_F$, and of the leading element, $V_{ud}$, of the Cabbibo-Kobayashi-Maskawa (CKM) matrix, see [4] for a recent review.

The $T=1/2$ mirror nuclei offer an alternative way to test the CVC hypothesis [3]. These nuclei decay via the mixed Fermi and Gamow-Teller (GT) transitions. Hence, apart from the radiative and the ISB theoretical corrections, the final values of $G_F$ and $V_{ud}$ depend on the ratio of statistical rate functions for the axial-vector and vector interactions, $f_A/f_V$, and the ratio of nuclear matrix elements $\rho \approx \lambda M_{GT}/M_F$ 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 a true constant $g_V=1$. The axial-vector current is partially conserved meaning that the coupling constant gets renormalized in nuclear medium. The effective axial-vector coupling constant, $g_A^{(\text{eff})} = g_A$, is quenched by an $A$-dependent factor, $q$, with respect to its free neutron decay value $g_A \approx -1.2701(25)$. Quenching factors deduced from comparisons between the large-scale nuclear-shell-model (NSM) calculations and experiment are: $q \approx 0.82$, $q \approx 0.77$ and $q \approx 0.74$ in the $p$-, $sd$-, and $pf$-shell, respectively. In heavier, $A=100$-$134$, nuclei, the average quenching is $q \approx 0.48$ [5]. This result is consistent, up to a theoretical uncertainty, with the result of Ref. [6]. Even stronger quenching, $g_A A^{-0.18}$, is used in the IBM-2 model [11].

The question about physical causes of the quenching has no unique answer. The quenching is usually related to: (i) missing correlations in the wave function, (ii) truncation of model space or (iii) to a very fashionable nowadays renormalization of the GT operator due to the two-body currents [11, 12]. Scenarios involving non-nucleonic degrees of freedom like $NN \to N\Delta$ excitations are shown to contribute only rather weakly [13].

Proper understanding of the quenching is essential for many branches of modern physics from modeling of astrophysical processes in stars to elusive neutrinoless double beta decay which depends on the fourth power of $g_A^{(\text{eff})}$ and is therefore particularly sensitive to $q$. In order to address the quenching, it is of paramount importance to investigate the GT matrix elements (MEs) using diverse theoretical models. The goal of this work is to communicate the pioneering application of the multi-reference density functional theory (MR-DFT) rooted no-core-configuration-interaction (NCCI) approach to study $\beta$-decay, with a particular emphasis on the GT process.
After a short introduction to the model we shall present the numerical results starting with the $\beta$-decay of $^8$He in order to test reliability of the model. Afterwards, the model will be applied to the sd- and lower pf-shell $T=1/2$ mirror nuclei, where both the GT MEs and the Fermi MEs will be computed.

The NCCI models rooted in MR-DFT offer nowadays an interesting alternative to the conventional nuclear shell model [14-17]. Firstly, they are capable of treating rigorously both the fundamental (spherical, particle number) as well as approximate (isospin) symmetries. Secondly, by invoking the generator coordinate method and/or mixing of discrete (quasi)particle-(quasi)hole (or particle-hole) configurations, they allow to incorporate important correlations into the nuclear wave function. Thirdly, they can be applied to any nucleus irrespectively of $A$ and the neutron and proton number parities. Moreover, by construction, they are able to capture core-polarization effects resulting from a subtle interplay between the long-range and short-range nucleon-nucleon forces, what is of critical importance for the calculation of isospin impurities and ISB corrections [17].

The NCCI formalism developed by our group [13-16] involves the angular momentum and isospin projections and subsequent mixing of states having good angular momentum and properly treated isospin. It proceeds in three distinct steps. First, we compute self-consistently a set of $k$ Hartree-Fock (HF) (multi)particle-(multi)hole configurations, $\{|\phi_j\rangle\}_j^{n=1}$, relevant for the problem under study. The Slater determinants $\{|\phi_j\rangle\}_j^{n=1}$ are calculated using true Skyrme interaction in order to avoid singularities at the next stage, at which we apply the angular momentum and isospin projections to determine, for each $j$, the family of states $\{|\phi_j; IMK; TT_z\rangle\}$ having good isospin $TT_z$, angular momentum $IM$, and angular-momentum projection on the intrinsic axis $K$. Subsequently, the states $\{|\phi_j; IMK; TT_z\rangle\}$ are mixed in order to account for the $K$ and isospin mixing. This gives a set of good angular-momentum states $\{|\phi_j; IM; T_z\rangle^{(i)}\}_i^{l=1}$ for each HF configuration $j$. The set is non-orthogonal and, in general, overcomplete. In the final step, the states are mixed over different configurations by solving the Hill-Wheeler-Griffin (HWG) equation, $\hat{H}u = ENu$, with the same Skyrme interaction that was used at the HF level. The HWG equation is solved in the collective space spanned by the natural states corresponding to non-zero eigenvalues $n$ of their norm matrix $N$. The same technique is used in the code to handle the $K$-mixing alone as described in detail in Ref. [18].

On exit, the NCCI code provides eigenfunctions that are labeled by the index $n$ numbering eigenstates in ascending order according to their energies and the strictly conserved quantum numbers $I$, $M$, and $T_z = (N - Z)/2$. The eigenstates can be decomposed in original projected (non-orthogonal) basis:

$$|n; IM; T_z\rangle = \sum_{i,j} a^{(n;IM;T_z)}_{ij} |\phi_j; IM; T_z\rangle^{(i)} \quad (1)$$

$$= \sum_{i,j, K,T \geq T_z} f^{(n;IM;T_z)}_{ijKT} \hat{P}^T_{T_zT_z} \hat{P}^I_{MK}|\phi_j\rangle,$$

where $\hat{P}^T_{T_zT_z}$ and $\hat{P}^I_{MK}$ stand for the isospin and angular-momentum projection operators, respectively. This form is particularly useful to compute MEs of the GT operator:

$$M_{\mu,\nu} = \mp \langle n'; IM'; T_z'|O_{\mu,\nu}|n; IM; T_z\rangle. \quad (2)$$

where $O_{\mu,\nu} = \frac{1}{\sqrt{2}} \sum_k \varepsilon^{(k)}_{1\mu} \sigma^{(k)}_{1\nu}$ is expressed by means of one-body spherical tensors. The isospin index above is fixed $\mu = \pm 1$ and it determines the overall phase factor. The matrix element (2) fulfills the Wigner-Eckart theorem:

$$M_{\mu,\nu} = \frac{1}{\sqrt{2T_{\mu} + 1}} C^{(n', IM', T_z')}_{M, IM, T_z} \langle n'; I' M' T_z'|O_{\mu,\nu}|n; I M T_z\rangle. \quad (3)$$

where $C^{(n', IM', T_z')}_{M, IM, T_z}$ stands for the Clebsch-Gordan coefficient. The reduced matrix element equals:

$$\langle n', I'|O_{\mu}|n, I\rangle = \mp \sum_{i,j, K,T \geq T_z} f^{(n'| I'M' T_z')}_{ijKT} f^{(n;IM;T_z)}_{ijKT} \sqrt{2T_{\mu} + 1} C^{(TT_z'T_z'|IKK')}_{TT_z T_z' IM IM', T_z T_z'} \sum_{\eta,\xi} C^{(1K)\xi}_{K\eta} C^{(T'T'|\xi,' \xi, j')}_{\xi,' \xi, j'} J^{(TT_z'T_z'|IKK')}_{\eta,\xi,\gamma, j'} \langle \gamma,\xi,\eta|O_{\mu} | \gamma,\xi,\eta\rangle. \quad (4)$$

The integral, $J$, runs over the beta Euler angle in isospace, $\beta_T$, and the Euler angles in space $\Omega = (\alpha, \beta, \gamma)$:

$$J^{(TT_z T_z'|IKK')}_{\eta,\xi,\gamma, j'} = \frac{2T_{\mu} + 1}{2} \int_0^\pi d\beta_T \sin \beta_T \int_0^\pi d\Omega \hat{D}^{(\kappa')}_{\kappa,\xi,\eta,\xi, j'} \langle \gamma,\xi,\eta|O_{\mu} | \gamma,\xi,\eta\rangle. \quad (5)$$

where $\hat{D}^{(\kappa')}_{\kappa,\xi,\eta,\xi, j'} = \frac{2I + 1}{2\pi^2} \int d\Omega \hat{D}^{(\kappa')}_{\xi,\xi,\kappa} \langle \phi_j|O_{\mu} | \phi_j\rangle$. The Wigner-Eckart relation [3] implies that the total probability of decay summed up over the components $\nu$ of the operator $O_{\mu,\nu}$ and over polarizations of the final state $M'$ is:

$$B(O_{\mu}; n, I \rightarrow n', I') = \frac{g^{2}_{A} |\langle n', I'|O_{\mu}|n, I\rangle|^2}{2I + 1} \equiv g^{2}_{A} \frac{|M_{GT}|^2}{2I + 1}. \quad (6)$$

The calculations discussed below were done using a new unpublished version of the HFODD solver [18, 19], which was equipped with the NCCI module. In order to
we have attempted to correlate the wave function of $^6$Li for the ground state (GS) of $^6$Li and determined the corresponding GT matrix element $|M_{GT}|=2.1645(43)$ assuming $g_A=-1.2701(25)$. This is an excellent test case for our model mainly because of a limited number of $ph$ configurations that can contribute in these $p$-shell nuclei. The results of the NCCI calculations performed for this transition is depicted in Fig. 1. The figure shows the calculated GT ME versus a number of configurations taken in the mixing. The very left point corresponds to a situation, where no mixing was performed in either of the nuclei. In this limit, called hereafter the MR-DFT limit, the HF reference states were selected based ultimately on the energy criterion. Note, that already in this limit the calculated ME is in fair agreement with the empirical value underestimating it by $\approx 7\%$. Next, keeping the wave function of $^6$He fixed, we have attempted to correlate the wave function of $^4$Li by admixing $1^+$ states projected from the lowest $ph$ configuration (second point) and from the first two lowest $ph$ configurations (third point). This caused an increase of the ME to 2.208 and 2.223, respectively, i.e. circa $3\%$ above the experiment, see Fig. 1. At this point we freeze the wave function of $^4$Li and attempt to correlate the wave function of $^6$He (last two points). This weakly influences the ME giving eventually 2.238. The test shows that the model is capable to capture main features of the wave functions that are important for reliable reproduction of the GT ME and provides stable predictions in function of a number of admixed configurations.

Recently, Knecht et al. [22] performed high-precision measurement of the $0^+\rightarrow1^+$ beta decay of $^6$He, which proceeds exclusively to the ground state (GS) of $^6$Li and determined the corresponding GT matrix element $|M_{GT}|=2.1645(43)$ assuming $g_A=-1.2701(25)$. This is an excellent test case for our model mainly because of a limited number of $ph$ configurations that can contribute in these $p$-shell nuclei. The results of the NCCI calculations performed for this transition is depicted in Fig. 1. The figure shows the calculated GT ME versus a number of configurations taken in the mixing. The very left point corresponds to a situation, where no mixing was performed in neither of the nuclei. In this limit, called hereafter the MR-DFT limit, the HF reference states were selected based ultimately on the energy criterion. Note, that already in this limit the calculated ME is in fair agreement with the empirical value underestimating it by $\approx 7\%$. Next, keeping the wave function of $^6$He fixed, we have attempted to correlate the wave function of $^4$Li by admixing $1^+$ states projected from the lowest $ph$ configuration (second point) and from the first two lowest $ph$ configurations (third point). This caused an increase of the ME to 2.208 and 2.223, respectively, i.e. circa $3\%$ above the experiment, see Fig. 1. At this point we freeze the wave function of $^4$Li and attempt to correlate the wave function of $^6$He (last two points). This weakly influences the ME giving eventually 2.238. The test shows that the model is capable to capture main features of the wave functions that are important for reliable reproduction of the GT ME and provides stable predictions in function of a number of admixed configurations.

![FIG. 1. (Color online) GT ME for beta decay of $^6$He in function of a number of configurations taken in the NCCI calculations in $^4$Li and $^6$He. Solid line shows the experimental value of Ref. [22].](image1)

Encouraged by the result obtained for the $^6$He decay, we have performed systematic study of the GT and Fermi MEs for the GS$\rightarrow$GS transitions in the $T=1/2$ mirror nuclei covering the $sd$- and lower $pf$-shell nuclei from $A=17$ till $55$. All results shown below were obtained using the SV$_{SO}$ EDF. This functional, apart from slightly more realistic s.p. levels, is also superior in reproducing binding energies (BE) in comparison to the SV EDF. The ability to reproduce masses is considered to be one of the most important signatures of the quality of DFT-rooted models. The calculated BE relative to empirical results are depicted in Fig. 2. Although the theory tends to overbind the lightest species and underbind the heavier, the overall agreement is at a quite impressive level of $\pm 1\%$. It is better almost by a factor of two than the level of agreement obtained for the SV interaction.

It appears also that the SV$_{SO}$ has reasonable spectroscopic properties. The theory is able to reproduce the GS spins already at the MR-DFT level with the exception of $A=19$ case, where the model predicts $I=5/2^+$ instead of $I=1^+/2$ to be the GS spin. The energy spectra are, in general, in fair agreement with data. For the sake of illustration Fig. 3 shows theoretical and experimental $I=3/2^+$ and $5/2^+$ states in the lower $sd$-shell nuclei. Similar agreement is obtained for heavier nuclei.

![FIG. 2. (Color online) Theoretical binding energies of $T=1/2$ mirror nuclei calculated using the NCCI framework. The results are shown relative to the experimental data.](image2)
els systematically overestimate the data beside the nuclei ranging from $A=29$ to 35. Strong suppression of the GT MEs in this mass range is related to aforementioned clustering of the $s_{1/2}$ and $d_{3/2}$ subshells in MF calculations. Proximity of these two subshells causes strong mixing, which has destructive impact on the calculated MEs. Comparison of the MR-DFT results obtained using the SV and SV$_{SO}$ EDFs supports this conclusion. Indeed, the MEs calculated using these two functionals are almost identical everywhere except for the mass region discussed above.

The Ikeda sum rule is an important indicator of the quality of theoretical models. For the $T=1/2$ mirrors it takes particularly simple form: $\sum_{n',I'} B(0^+; n, I \to n', I') = 3$. Systematic study of the Ikeda sum rule with the present formalism involving the isospin and angular momentum projections is CPU expensive. Hence, it was limited here to one of the simplest cases of $A=39$ nuclei. In this case, inclusion of all possible $ph$ excitations within the $sd$-shell exhausts 99% of the sum rule as illustrated in Fig. 6. It is worth mentioning that inclusion of $ph$ excitations between the spin-orbit partners $d_{5/2} \to d_{3/2}$ is crucial for the sum rule. More systematic study of the sum rules will be done with the variant involving only the angular momentum projection.

The use of NCCI approach involving both the isospin and angular momentum projected states is absolutely necessary to study Fermi transitions and, in particular, to extract the ISB corrections to the Fermi branch of $\beta$-decay. Let us recall that the ISB corrections are needed to study the CVC hypothesis and the CKM matrix via the transitions in the mirrors, see Ref. [5]. The results obtained in this study are collected in Tab. I. It is bene-
In summary, we have presented a systematic study of the GS→GS GT and Fermi MEs in $T=1/2$ mirror nuclei using, for the first time, the NCCI approach based on the isospin and angular momentum projected MR-DFT formalism. The framework is universal and can be applied to any nucleus irrespectively on its mass and the proton and neutron number parities. It can be also improved and optimized in many different ways, in particular, concerning the tensor force which is known to have an impact on the shell structure and β-decay.

In the present implementation with the SV or SVSO EDFs the calculated GT MEs systematically overestimate experimental data for the free neutron strength of the axial current. The level of disagreement is found to be very similar to the one obtained using large scale shell model in spite of the fundamental differences between the two approaches in handling the core and the core polarization effects, the correlations or the basis truncation. It strongly suggests, that the mechanism of in-medium renormalization of the axial strength may indeed be related to the two-body currents. This conjecture requires further studies.

Eventually, we have also calculated the ISB corrections to the Fermi decay branch in the $T=1/2$ mirror nuclei. The corrections turn out to be in a very good agreement with the NSM calculations.

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![Graph showing the total binding energy of 39Ca.](image)

**Fig. 6.** (Color online) Ikeda sum rule for the GS of 39Ca. Thick horizontal lines indicate the theoretical (solid) and experimental (dashed) total BE of the GS in 39Ca and the lowest 1/2+, 3/2+, and 5/2+ states in 39K. The numbers over the arrows indicate the total calculated GT strength for each $I$. Multiple arrows and shadowing indicate that the strength is distributed over several states.

**TABLE I.** Theoretical ISB corrections, $\delta_C^{(NCCI)}$, (in %) adopted in this work. For the sake of comparison the table contains also the NSM results, $\delta_C^{(NSM)}$, of Ref. [24].

| A  | $\delta_C^{(NCCI)}$ | $\delta_C^{(NSM)}$ | A  | $\delta_C^{(NCCI)}$ | $\delta_C^{(NSM)}$ |
|----|----------------------|---------------------|----|----------------------|---------------------|
| 17 | 0.166(17)            | 0.585(27)           | 37 | 0.907(91)            | 0.734(61)           |
| 19 | 0.339(34)            | 0.415(39)           | 39 | 0.318(32)            | 0.855(81)           |
| 21 | 0.300(30)            | 0.348(27)           | 41 | 0.426(43)            | 0.87(12)            |
| 23 | 0.316(32)            | 0.293(22)           | 43 | 0.690(69)            | 0.50(10)            |
| 25 | 0.439(44)            | 0.312(34)           | 45 | 0.589(59)            | 0.87(12)            |
| 27 | 0.520(52)            | 0.976(53)           | 47 | 0.673(67)            | 0.673(67)           |
| 29 | 0.585(59)            | 0.715(36)           | 49 | 0.646(65)            | 0.646(65)           |
| 31 | 0.705(71)            | 0.865(59)           | 51 | 0.714(71)            | 0.714(71)           |
| 33 | 0.366(37)            | 0.493(46)           | 53 | 0.898(90)            | 0.898(90)           |
| 35 | 0.366(37)            | 0.493(46)           | 55 | 0.620(62)            | 0.620(62)           |

Official to see that our corrections are very consistent with the NSM results of Ref. [24].