Isospin mixing within the multi-reference nuclear density functional theory and beyond - selected aspects

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The results of systematic calculations of isospin-symmetry-breaking corrections to superallowed $\beta$-decays based on the self-consistent isospin- and angular-momentum-projected nuclear density functional theory (DFT) are reviewed with an emphasis on theoretical uncertainties of the model. Extensions of the formalism towards no core shell model approach with basis cutoff scheme dictated by the self-consistent particle-hole DFT solutions will be also discussed.

I. INTRODUCTION

Isospin symmetry in atomic nuclei is weakly broken mostly by the Coulomb interaction that exerts a long-range polarization effect. Capturing an equilibrium between long and short range effects is a challenging task possible only within no core approaches, which, in heavier nuclei, reduces possible choices to formalisms rooted in the density functional theory (DFT). However, as it was recognized already in the 70’s [1], the self-consistent mean-field (MF) approaches cannot be directly applied to compute isospin impurities because of spurious mixing caused by the spontaneous symmetry breaking (SSB) effects. This observation hindered theory from progress in the field for decades.

The aim of this work is to present a brief overview of recent theoretical results obtained within the isospin- and angular-momentum projected DFT on isospin-mixing effects. Our multi-reference no core DFT was specifically designed to treat rigorously the conserved rotational symmetry and, at the same time, tackle the explicit breaking of the isospin symmetry due to the Coulomb field. The major physics motivation behind developing the model and studying the isospin symmetry breaking (ISB) comes from nuclear beta decay. Theoretical corrections to the superallowed Fermi beta decay matrix elements $I = 0^+, T = 1 \rightarrow I = 0^+, T = 1$ between the isobaric analogue states, caused by the ISB, are critical for precise determination of the leading element $V_{ud}$ of the Cabibbo-Kobayashi-Maskawa (CKM) flavour-mixing matrix and, in turn, for further stringent tests of its unitarity, violation of which may signalize new physics beyond the Standard Model of particle physics, see [2] and refs. quoted therein.

II. MULTI-REFERENCE DENSITY FUNCTIONAL THEORY

The formalism employed here starts with the self-consistent Slater determinant $|\varphi\rangle$ obtained by solving Skyrme-Hartree-Fock equations without pairing. The state violates both the rotational and isospin symmetries. The strategy is to restore the rotational invariance, remove the spurious isospin mixing caused by the isospin SSB effect, and retain only the physical isospin mixing due to the electrostatic interaction [3]. This is achieved by a rediagonalization of the entire Hamiltonian, consisting the isospin-invariant kinetic energy and Skyrme force and the isospin-non-invariant

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Coulomb force, in a basis that conserves both angular momentum and isospin $|\varphi; IMK; TT_z\rangle$, projected from the state $|\varphi\rangle$:

$$|\varphi; IMK; TT_z\rangle = \frac{1}{\sqrt{N_{\varphi;IMK;TT_z}}} \hat{P}_{T_z}^{\dagger} \hat{P}_{M,K}^{\dagger} |\varphi\rangle,$$

where $\hat{P}_{T_z}^{\dagger}$ and $\hat{P}_{M,K}^{\dagger}$ stand for the standard isospin and angular-momentum projection operators [4], respectively. One must also treat the fact that the quantum number $K$ is not conserved and set (1) is overcomplete. This requires selecting the subset of linearly independent states, known as collective space [4], which is spanned, for each $I$ and $T$, by the so-called natural states $|\varphi; IM; TT_z\rangle^{(i)}$ [5] and subsequently rediagonalizing the entire Hamiltonian in the collective space. The resulting eigenfunctions are:

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

where index $n$ labels the eigenstates in ascending order of energies.

### III. ISOSPIN MIXING

The isospin or Coulomb impurities are defined as:

$$\alpha_C^N = 1 - \sum_{i} |a_{iTT}^{(n;\varphi)}|^2,$$

where the sum extends over the norms corresponding to isospin $T$ that dominates in wave function (2).

It is well known that for modern density-dependent Skyrme and Gogny energy density functionals (EDFs), the angular momentum projection is ill-defined [9, 10]. Hence, at present, the double-projected DFT method can be safely used only with the functionals originating from the true Hamiltonian. Nevertheless, for all modern Skyrme forces, the isospin-only-projected variant of the approach is free from singularities [3]. Fig. 4 shows the isospin impurities in the ground-states of even-even $N = Z$ nuclei, calculated by using the state-of-the-art SLy4 Skyrme [6] EDF in the isospin-only-projected variant of the model [3, 11]. It is gratifying to see that the calculated impurities are consistent with the recent data extracted from the giant-dipole-resonance decay studies in $^{80}$Zr [8] and isospin-forbidden E1 decay in $^{64}$Ge [7], see Fig. 4. Both data points disagree with the pure MF results, which, due to the spurious mixing caused by the spontaneous ISB effects, are lower by almost $\sim 30\%$. The agreement with available data indicates that the model is capable of quantitatively capturing the intensity of the isospin mixing. This is important in the context of performing reliable calculations of the ISB corrections to the Fermi beta decay.

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**Fig. 1:** Isospin impurities in even-even $N = Z$ nuclei calculated by using the SLy4 Skyrme EDF [6]. Full triangles mark the values calculated by using the isospin-projected DFT. Open triangles show mean-field values that are artificially quenched by the spurious isospin mixing. Stars mark empirical results in $^{64}$Ge [7] and $^{80}$Zr [8].
IV. ISOSPIN-SYMMETRY-BREAKING CORRECTIONS TO THE SUPERALLOWED FERMI BETA DECAY

The $0^+ \rightarrow 0^+$ Fermi $\beta$-decay proceeds between the ground state ($g.s.$) of the even-even nucleus ($I = 0, T \approx 1, T_z = \pm 1$) and its isospin-analogue partner in the $N = Z$ odd-odd nucleus, ($I = 0, T \approx 1, T_z = 0$). Since the isospin projection alone leads to unphysically large isospin mixing in odd-odd $N = Z$ nuclei \[11\], to calculate Fermi matrix elements the double-projected method must be applied. As already mentioned, the angular momentum projection brings back the singularities in the energy kernels \[11\], preventing one from using the modern parametrizations of the Skyrme EDFs and forcing us to use the Hamiltonian-driven Skyrme SV EDF \[12\].

The g.s. of the even-even parent nucleus is approximated by the state $|\psi; I = 0, T \approx 1, T_z = \pm 1\rangle$, projected from the Slater determinant $|\psi\rangle$ representing the self-consistent g.s. MF solution, which is unambiguously defined by filling in the pairwise doubly degenerate levels of protons and neutrons up to the Fermi level.

The odd-odd daughter state is approximated by the state $|\varphi; I = 0, T \approx 1, T_z = 0\rangle$, projected from the self-consistent Slater determinant $|\varphi\rangle \equiv |\bar{\nu} \otimes \pi\rangle$ (or $|\nu \otimes \bar{\pi}\rangle$) representing the so-called anti-aligned MF configuration, obtained by placing the odd neutron and odd proton in the lowest available time-reversed (or signature-reversed) single-particle orbits. The isospin projection from Slater determinants manifestly breaking the isospin symmetry is essentially the only way to reach the $T \approx 1$ states in odd-odd $N = Z$ nuclei that are beyond the MF model space.

This allows for rigorous fully quantal evaluation of the beta-decay transition matrix element and the corresponding ISB correction $\delta_C$:

$$|M_F^{(\pm)}|^2 = |\langle \psi; I = 0, T \approx 1, T_z = \pm 1|\bar{T}_\pm|\varphi; I = 0, T \approx 1, T_z = 0\rangle|^2 \equiv 2(1 - \delta_C).$$

The calculated ISB corrections $\delta_C$ lead to $|V_{ud}| = 0.97397(27)$ and $|V_{ud}| = 0.97374(27)$, for the SV and SHZ2 EDFs, respectively \[12\]. Both values result in the unitarity of the CKM matrix up to 0.1%. The new parametrization SHZ2 has been specifically developed to assess the robustness of our results with respect to the choice of interaction. This shows that although individual ISB corrections are sensitive to the interplay between the bulk symmetry energy and time-odd mean-fields, the value of $|V_{ud}|$ rather weakly depends on the parametrization. It is gratifying to see that our results are fully consistent with the results obtained by Towner and Hardy \[13\], which were obtained within a different methodology, based on the nuclear shell-model combined with mean-field wave functions. Both approaches disagree with the RPA-based study of Ref. \[14\]. The theoretical results are summarized in Fig. 2.
FIG. 3: Low-lying low-spin $I = 0, 1, 2$ states in $^{32}$Cl. Solid lines show theoretical levels obtained by mixing states projected from nine low-lying self-consistent particle-hole configurations. Dashed lines mark experimental data [19]. Note that spin assignments of, in particular, $2^+$ states are uncertain. The spectra have been normalized to the lowest $1^+$ state.

V. OUTLOOK: BEYOND THE MULTI-REFERENCE DFT

Implementation of the theory that we presented above was based on a projection from a single Slater determinant, which, in odd-odd daughter nucleus, was not uniquely defined. At present, we are implementing an extended version of the model, which allows for mixing of states projected from different self-consistent Slater determinants representing low-lying (multi)particle-(multi)hole excitations in a given nucleus. Such an extension can be viewed as a variant of no core shell-model with two-body effective interaction (including the Coulomb force) and a basis truncation scheme dictated by the self-consistent deformed Hartree-Fock solutions. Preliminary spectrum of low-spin $I = 0, 1, 2$ states in $^{32}$Cl obtained by mixing states projected from nine low-lying particle-hole configurations is shown in Fig. 3. In spite of certain technical problems related to divergencies, which will be discussed elsewhere, the results are very encouraging. This is particularly the case in view of the fact that the self-consistent states and their mixing were determined by using the SV Skyrme EDF, which has rather poor spectroscopic properties.

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