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Beta-decay Studies in $N \approx Z$ Nuclei Using No-Core Configuration-Interaction Model

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The no-core configuration-interaction model based on the isospin- and angular-momentum projected density functional formalism is introduced. Two applications of the model are presented: (i) determination of spectra of 0^+ states in ^{62}Zn and (ii) determination of isospin-symmetry-breaking corrections to superallowed β -decay between isobaric-analogue 0^+ states in ^{38}Ca and ^{38}K . It is shown that, without readjusting a single parameter of the underlying Skyrme interaction, in all three nuclei, the model reproduces the 0^+ spectra surprisingly well.

KEYWORDS: density functional theory, configuration-interaction model, superallowed Fermi β -decay, isospin symmetry breaking

1. Introduction

Superallowed Fermi β -decays between the isobaric analogue states, $[I = 0^+, T = 1] \rightarrow [I = 0^+, T = 1]$, provide the most precise values of the vector coupling constant G_V and leading element V_{ud} of the Cabibbo-Kobayashi-Maskawa (CKM) flavour-mixing matrix, which are critical for stringent tests of weak-interaction flavor-mixing sector of the Standard Model of particle physics. In particular, these data are needed for testing unitarity of the CKM matrix, violation of which may signalize *new physics* beyond the Standard Model, see [1] and refs. quoted therein.

In testing the Standard Model, precision is of utmost importance. Only the β -decays, for which the reduced life-times, ft , are measured with accuracy better than half a percent, can be used for that purpose. At present, thirteen such cases are known in nuclei, ranging in mass from $A=10$ to $A=74$. The extraction of G_V and V_{ud} is not solely dependent on experimental data but also requires theoretical input in the form of radiative and many-body corrections to the experimental ft values. The corrections are small, of the order of a percent, but are critical for the applicability of the entire method, because it relies on the so-called conserved vector current hypothesis (CVC). The CVC hypothesis assumes independence of the vector current on nuclear medium, and must be verified *a priori* by investigating mass independence of the corrected reduced life-times defined as:

$$\mathcal{F}t \equiv ft(1 + \delta'_R)(1 + \delta_{\text{NS}} - \delta_C) = \frac{K}{2G_V^2(1 + \Delta_R^V)} \approx \text{const.}, \quad (1)$$

where $K/(\hbar c)^6 = 2\pi^3 \hbar \ln 2/(m_e c^2)^5 = 8120.2787(11) \times 10^{-10} \text{ GeV}^{-4} \text{ s}$ is a universal constant. Symbols δ'_R , δ_{NS} , Δ_R^V are the radiative corrections while δ_C stands for the isospin symmetry-breaking (ISB) correction to the Fermi matrix element:

$$|M_F^{(\pm)}|^2 = |\langle I = 0^+, T \approx 1, T_z = \pm 1 | \hat{T}_\pm | I = 0^+, T \approx 1, T_z = 0 \rangle|^2 = 2(1 - \delta_C). \quad (2)$$

Since the isospin symmetry is weakly broken, mostly by the Coulomb interaction that polarizes the entire nucleus, microscopic calculation of the ISB corrections is a challenging task. Capturing a delicate equilibrium between the hadronic and Coulomb effects is fully possible only within *no core* approaches. This, in heavier nuclei, reduces the possible choices to formalisms rooted in the density functional theory (DFT). However, as it was recognized already in the 70's [2], to determine the magnitude of isospin impurities, the self-consistent mean-field (MF) approaches cannot be directly applied, because of a spurious mixing caused by the spontaneous symmetry-breaking effects. This observation hindered theory from progress in the field for decades.

To overcome these problems, over the last few years we have developed a no-core multi-reference DFT, which involves the isospin- and angular-momentum projections of Slater determinants representing the 0^+ triplet states in mother and daughter nuclei [3, 4]. The formalism, dubbed static, 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. Recently, by allowing for mixing of states that are projected from self-consistent Slater determinants representing low-lying (multi)particle-(multi)hole excitations, we have extended the model to the so-called dynamic variant [5]. The model belongs to the class of the *no core* configuration-interaction approaches, with the two-body short-range (hadronic) and long-range (Coulomb) interactions treated on the same footing. It is based on a truncation scheme dictated by the self-consistent deformed Hartree-Fock (HF) solutions. The model can be used to calculate spectra, transitions, and β -decay matrix elements in any nuclei, irrespective of their mass and neutron- and proton-number parities.

The aim of this work is to present this novel theoretical framework along with preliminary results for the low-spin spectra and β -decay matrix elements in selected $N \approx Z$ nuclei. The first applications of the model to the low-lying spectra in ^{32}Cl and ^{32}S have been published in [5]. Hereafter, we focus on nuclei relevant to high-precision tests of the weak-interaction flavor-mixing sector of the Standard Model. In this perspective, we discuss the spectrum of 0^+ states in ^{62}Zn , which was reassigned in a recent experiment [6], and is now posing a challenge to theory. We also briefly overview preliminary attempts and difficulties arising in determining the ISB correction to the superallowed $^{62}\text{Ga} \rightarrow {}^{62}\text{Zn}$ $0^+ \rightarrow 0^+$ β -decay, which is strongly model dependent. We also present preliminary results for the ISB correction to the Fermi matrix element corresponding to the $^{38}\text{Ca} \rightarrow {}^{38}\text{K}$ transition. In our static calculations, the case of $A=38$ was excluded from the canonical pool of superallowed data. This was because of the anomalously large ISB correction, caused by uncontrolled mixing of the $2s_{1/2}$ and $1d_{3/2}$ orbits, which for the SV_T Skyrme *true* interaction are almost degenerate. The SV_T interaction is the SV functional [7] augmented with the tensor terms, see discussion in [8].

The paper is organized as follows. In Sec. 2, the basics of our dynamical model are briefly sketched. In Sec. 3, preliminary numerical results concerning spectrum of 0^+ states in ^{62}Zn and the ISB corrections for $^{38}\text{Ca} \rightarrow {}^{38}\text{K}$ Fermi transitions are presented. The paper is summarized in Sec. 4.

2. No-core configuration-interaction model

The static variant of our model is based on the double projection, on isospin and angular momentum, of a single Slater determinant. In an even-even nucleus, the Slater determinant representing the ground-state is uniquely defined. In an odd-odd nucleus, the conventional MF theory that gives Slater determinants separately for neutrons and protons faces problems. First, there is no single Slater determinant representing the $I = 0^+, T = 1$ state, see [4, 9]. In our approach, this obstacle is removed by projecting from the so-called anti-aligned Slater determinant. This configuration, by construction, has no net alignment and manifestly breaks the isospin symmetry, being an almost fifty-fifty mixture of the $T = 0$ and $T = 1$ states. In this way, the needed $T = 1$ component can be recovered. The problem is, however, that the anti-aligned states are not uniquely defined. In the general case of a triaxial nucleus, there exist three linearly-dependent Slater determinants, built of valence neutron and

proton single-particle states that carry angular momenta aligned along the X ($|\varphi^{(X)}\rangle$), Y ($|\varphi^{(Y)}\rangle$), or Z ($|\varphi^{(Z)}\rangle$) axes of the intrinsic frame of reference or, respectively, along the long, intermediate, and short axes of the core. In our calculations, no tilted-axis anti-aligned solution was found so far.

In the static approach, the only way to cope with this ambiguity is to calculate three independent β -decay matrix elements and to take the average of the resulting δ_C values. Such a solution is not only somewhat artificial, but also increases the theoretical uncertainty of the calculated ISB corrections. This deficiency motivated our development of the dynamic model, which allowed for mixing states projected from the three reference states $|\varphi^{(k)}\rangle$ for $k=X, Y$, and Z , with the mixing matrix elements derived from the same Hamiltonian that was used to calculate them. The dynamic model further evolved towards a full no-core configuration-interaction (NCCI) model, in which we allow for mixing states projected from different low-lying (multi)particle-(multi)hole Slater determinants $|\varphi_i\rangle$. This final variant has all features of the *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.

The computational scheme proceeds in four major steps:

- First, a set of relevant low-lying (multi)particle-(multi)hole HF states $\{\varphi_i\}$ is calculated along with their HF energies $e_i^{(\text{HF})}$, which form a subspace of reference states for subsequent projections.
- Second, the projection techniques are applied to the set of states $\{\varphi_i\}$, so as to determine the family of states $\{\Psi_{TIK}^{(i)}\}$ having good isospin T , angular momentum I , and angular-momentum projection on the intrinsic axis K .
- Third, states $\{\Psi_{TIK}^{(i)}\}$ are mixed, so as to properly take into account the K mixing and Coulomb isospin mixing – this gives the set of good angular-momentum states $\{\Psi_I^{(i)}\}$ of the static model [3, 4].
- Finally, the mixing of, in general, non-orthogonal states $\{\Psi_I^{(i)}\}$ for all configurations i is performed by solving the Hill-Wheeler equation in the collective space spanned by the natural states corresponding to non-zero eigenvalues of their norm matrix, that is, by applying the same technique, which was used to handle the K -mixing alone [10].

The numerical stability of the method is affected by necessary truncations of the model space, namely, numerically unstable solutions are removed by truncating either the high-energy states $\{\Psi_I^{(i)}\}$ or the *natural states* corresponding to small eigenvalues of the norm matrix, or by applying both truncations simultaneously. Although such truncation procedure gives reliable values of the energy, the results shown below must still be considered as preliminary.

3. Numerical results

The CKM matrix element $|V_{ud}| = 0.97397(27)$ obtained with a set of the ISB corrections calculated using the double-projected DFT method [4] agrees very well with the result obtained by Towner and Hardy (TH) [11], $|V_{ud}| = 0.97418(26)$, obtained within methodology based on the nuclear shell-model combined with Woods-Saxon mean-field (SM+WS) wave functions. Both values result in the unitarity of the CKM matrix up to 0.1%. It is gratifying to see that also individual DFT values of δ_C are consistent within 2σ with the values calculated in Ref. [11] (see Fig. 7 of Ref. [4]). This holds up to three exceptions of the ISB corrections to ${}^{10}\text{C} \rightarrow {}^{10}\text{B}$, ${}^{38}\text{K} \rightarrow {}^{38}\text{Ar}$, and ${}^{62}\text{Ga} \rightarrow {}^{62}\text{Zn}$ transitions. The two latter mass numbers, more precisely transitions ${}^{38}\text{Ca} \rightarrow {}^{38}\text{K}$ and ${}^{62}\text{Ga} \rightarrow {}^{62}\text{Zn}$, are analyzed below using the newly developed NCCI approach. It is worth mentioning here that the mutually consistent DFT and TH results are at variance with the RPA-based study of Ref. [12], which gives systematically smaller values of δ_C and, in turn, considerably smaller value of matrix element V_{ud} .

3.1 No-core configuration-interaction calculations for 0^+ states in ^{62}Zn

A large difference between the ISB corrections to the $^{62}\text{Ga} \rightarrow {}^{62}\text{Zn}$ Fermi matrix element, calculated using the DFT and SM+WS approaches, is one of the motivations to undertake the NCCI studies of the participating nuclei. Interestingly, nucleus ^{62}Zn has been recently remeasured by the TRIUMPH group [6], and its spectrum of low-lying 0^+ states is now posing a great challenge to theory, as shown in the Tab. I and Fig. 1. Both the table and figure also include results of our NCCI study, which involves the mixing of 0^+ states projected from six reference states. They comprise the deformed ground state (g.s.) and five low-lying excited HF configurations, including two lowest proton (π_1 and π_2) and two lowest neutron (ν_1 and ν_2) p-h excitations, and the lowest proton-proton 2p-2h configuration, all calculated with respect to the g.s.

Table I. Excitation energies of 0^+ states in ^{62}Zn up to 5 MeV. First two columns show old and new experimental data, see [6] for details. Next three columns collect the results of shell-model calculations using MSDI3 [13], GXPF1 [14], and GXPF1A [15] interactions, respectively. Last column shows the results obtained in this work using six reference Slater determinants described in the text. All values are in keV.

OLD	NEW	MSDI3	GXPF1	GXPF1A	SV ^{mix}
2341.95(2)		2263	2320	2094	
		2874		2811	
3042.9(8)	3045.5(4)	3071		3457	2953
	3862(2)	3513	3706	3682	3884
4008.4(7)	3936(6)	3833		3991	4263
				4444	
4620(20)	4552(9)	4551	4729	4643	4347

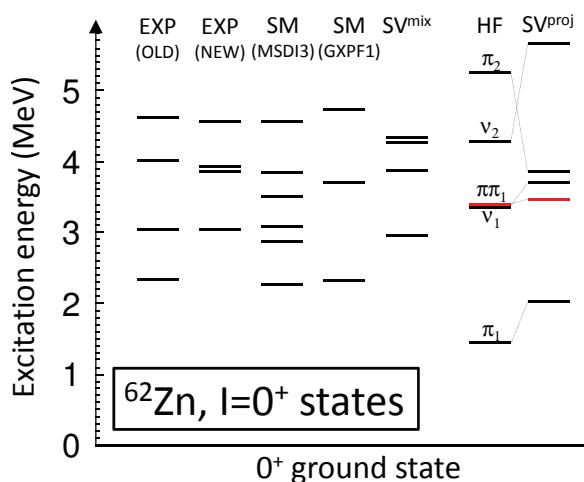


Fig. 1. The first five columns show low-energy $I=0^+$ states in ^{62}Zn listed in Table I. Columns marked HF and SV^{proj} show MF results obtained for the six HF configurations and those for the 0^+ states projected from the HF configurations before the mixing, respectively.

It is gratifying to observe that our model is able to capture, without adjusting a single parameter, the spectrum of 0^+ states in ^{62}Zn very accurately, even better than the state-of-the-art SM calculations. Moreover, as shown in Fig. 2, the calculated spectrum of the 0^+ states in ^{62}Zn is relatively stable with

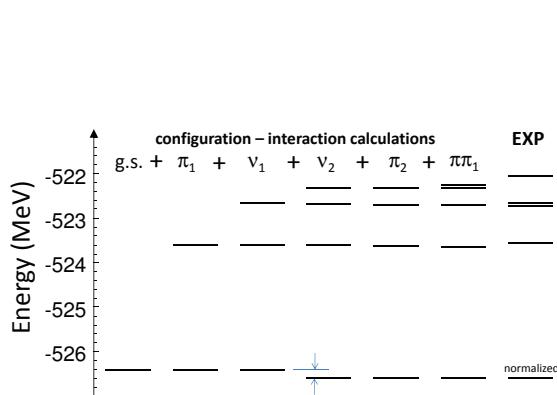


Fig. 2. Stability of the absolute energies of the calculated 0^+ states in ^{62}Zn with respect to number of reference configurations included in the calculations.

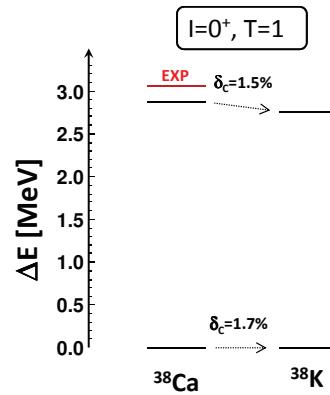


Fig. 3. Calculated energies of the 0_2^+ relative to 0_1^+ states in ^{38}Ca and ^{38}K , and the ISB corrections to the corresponding $0_1^+ \rightarrow 0_1^+$ and $0_2^+ \rightarrow 0_2^+$ transitions. Empirical excitation energy of the 0_2^+ state in ^{38}Ca is also shown.

respect to increasing the number of reference configurations. The last two columns of Fig. 1 illustrate the importance of symmetry restoration and configurations mixing.

Unfortunately, the calculated corrections δ_C are sensitive to tiny admixtures to the wave function and, and present, the calculated values are not stable. For example, by adding the 0^+ state projected from configuration ν_2 , one changes the absolute g.s. energy of ^{62}Zn by only $\approx 200\text{keV}$, but at the same time δ_C changes by $\approx 4\%$. Such a large change of δ_C is probably entirely artificial, reflecting the fact that the spaces of states used to calculate the parent and daughter nuclei do not match.

3.1.1 ISB correction to $^{38}\text{K} \rightarrow ^{38}\text{Ca}$ transition

In the static DFT calculations, the ISB correction to the $^{38}\text{K} \rightarrow ^{38}\text{Ar}$ and $^{38}\text{Ca} \rightarrow ^{38}\text{K}$ superallowed transitions turned out to be unphysically large [3], and were disregarded. The reason could be traced back to unphysical values of the single-particle (s.p.) energies of the $2s_{1/2}$ and $1d_{3/2}$ orbits, which, for the SV functional, in the double magic nucleus ^{40}Ca are almost degenerate and can therefore strongly mix, in particular through the time-odd fields in odd-odd ^{38}K . To gain a better insight into the problem, in this work we perform the NCCI study of both nuclei, ^{38}K and ^{38}Ca . For our preliminary results presented in this work, we were able to converge three low-lying antialigned reference configurations in ^{38}K and four configurations in ^{38}Ca . Their basic properties, including labels in terms of the dominant Nilsson components of the hole orbitals, are listed in Table II.

Results of our NCCI calculations, giving energies of the 0^+ states and the corresponding ISB corrections to β -decays, are visualized in Fig. 3. Again, our model accurately reproduces the experimental excitation energy of the second 0_2^+ state in ^{38}Ca . Indeed, the measured value, $\Delta E_{\text{EXP}} = 3057(18)$ keV, is only 186 keV higher than the calculated one, $\Delta E_{\text{TH}} = 2871$ keV. The ISB corrections to the $^{38}\text{Ca} \rightarrow ^{38}\text{K}$ transitions are for $0_1^+ \rightarrow 0_1^+$ and $0_2^+ \rightarrow 0_2^+$ equal to 1.7% and 1.5%, respectively. As compared to the static theory, which for the 0_1^+ states gives $\delta_C = 8.9\%$, these values are strongly reduced, but they are almost twice larger than the result of TH [11], who quote $\delta_C = 0.745(70)\%$.

Let us finally mention that the calculated energies of 0_2^+ relative to 0_1^+ states in ^{38}Ar and ^{38}K (preliminary value resulting from mixing of 0^+ states projected from three HF configurations) are $\Delta E_{\text{TH}} = 2757$ keV and $\Delta E_{\text{TH}} = 3161$ keV, respectively. The latter value is in very good agreement with the experimental relative energy equal to $\Delta E_{\text{EXP}} = 3377.45(12)$ keV.

Table II. Properties of reference Slater determinants in ^{38}K and ^{38}Ca nuclei, including their excitation energies, valence particle alignments in odd-odd nucleus ^{38}K and their orientations, quadrupole moments, and triaxiality. The determinants are labeled by Nilsson quantum numbers $[N, n_z, \Lambda, \Omega]$ pertaining to dominant components of the hole states.

k	$ ^{38}\text{K}; k\rangle$	ΔE_{HF} (MeV)	j_ν/j_π	Q_2 (fm 2)	γ ($^\circ$)	$ ^{38}\text{Ca}; k\rangle$	ΔE_{HF} (MeV)	Q_2 (fm 2)	γ ($^\circ$)
1	$ 202\frac{3}{2}\rangle^{-2}$	0.000	-0.50/0.50(Y)	0.44	60	$ 200\frac{1}{2}\rangle^{-2}$	0.000	0.47	60
2	$ 220\frac{1}{2}\rangle^{-2}$	1.380	0.50/-0.50(Z)	0.18	0	$ 200\frac{1}{2}\rangle^{-2}$	0.762	0.03	0
3	$ 211\frac{1}{2}\rangle^{-2}$	1.559	-1.50/1.50(Z)	0.22	0	$ 211\frac{1}{2}\rangle^{-2}$	1.669	0.24	0
4						$ 220\frac{1}{2}\rangle^{-1} \otimes 202\frac{3}{2}\rangle^{-1}$	2.903	0.09	60

4. Summary

We presented a novel no-core configuration-interaction approach, which is based on mixing the isospin- and angular-momentum-projected deformed DFT configurations. The model is specifically tailored to determining the low-lying spectra and β -decay transitions in $N \approx Z$ nuclei, where the isospin degree of freedom is essential. The model can be viewed as a variant of the no-core shell model. Its advantage over the standard shell model formulation is that it can be applied, at least in principle, to any nucleus of arbitrary mass and number parity.

Two applications of the model, both relevant to studies of superallowed Fermi β decays, were presented. The model has been used to compute the 0^+ spectrum of ^{62}Zn and ISB corrections to the Fermi β decays between the $0_1^+ \rightarrow 0_1^+$ and $0_2^+ \rightarrow 0_2^+$ isobaric analogue states in ^{38}Ca and ^{38}K . We demonstrated that without adjusting any single parameter, it well reproduces the spectra of 0^+ states. Predictions for the ISB corrections appear to be, at least at present, somewhat less reliable. The reason is that the isospin mixing is a very subtle effect, requiring a perfect matching of spaces of states used in the parent and daughter nuclei, which is difficult to achieve in practice. Work toward improving this aspect of the model is in progress.

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