Isospin mixing in nuclei within the nuclear density functional theory

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We present the self-consistent, non-perturbative analysis of isospin mixing using the nuclear density functional approach and the rediagonalization of the Coulomb interaction in the good-isospin basis. The largest isospin-breaking effects are predicted for $N=Z$ nuclei and they quickly fall with the neutron excess. The unphysical isospin violation on the mean-field level, caused by the neutron excess, is eliminated by the proposed method. We find a significant dependence of the magnitude of isospin breaking on the parametrization of the nuclear interaction term. A rough correlation has been found between the isospin mixing parameter and the difference of proton and neutron rms radii. The theoretical framework described in this study is well suited to describe a variety of phenomena associated with isospin violation in nuclei, in particular the isospin symmetry-breaking corrections to superallowed Fermi beta decays.

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The isospin symmetry, introduced by Heisenberg [1] and Wigner [2], is largely preserved by strong interactions; a small violation of isospin on the hadronic level is due to the difference in the masses of the up and down quarks [3]. In atomic nuclei, the main source of isospin breaking is the electromagnetic interaction [4, 5]. Since the isovector and isotensor parts of electromagnetic force are much weaker than the strong interaction between nucleons, many effects associated with isospin breaking in nuclei can be treated in a perturbative way. With this caveat, the formalism of isotopic spin is a very powerful concept in nuclear structure and reactions [6, 7], where many spectacular examples of isospin symmetry can be found.

The main effect of Coulomb force in nuclei is to exert a long-range overall polarization effect on nuclear states whose detailed structure is dictated by the short-ranged strong force. The net effect of such a polarization is a result of two competing trends: the nuclear force is strongly attractive in the isoscalar neutron-proton channel, while the Coulomb force acts against this attraction by making neutron and proton states different. In order to explain this interplay, self-consistent feedback between strong and electromagnetic fields must be considered to best locate the point of the nuclear equilibrium.

An excellent example of this interplay is the systematic behavior of nuclear binding energies: with increasing mass number, the stability line bends away from the $N=Z$ line towards the neutron-rich nuclei. The effect of electromagnetic force on nuclear binding is clearly non-perturbative. Even in medium-mass nuclei, which are of principal interest in this study, energy balance between strong and Coulomb forces is not tremendously favorable, e.g., 342 MeV versus 72 MeV in $^{40}$Ca. The situation becomes dramatic in superheavy nuclei and in the neutron star crust, where not only the binding but also spectra are strongly impacted by the Coulomb frustration effects resulting from a self-consistent, non-perturbative feedback between strong and electromagnetic parts of the nuclear Hamiltonian [8, 9].

The strong motivator for studies of isospin breaking is nuclear beta decay. The new data in superallowed $0^+\rightarrow0^+$ beta decays [10], including a number of high-precision Penning-trap measurements, require improved calculations of isospin-breaking corrections [11, 12]. As far as nuclear spectroscopy is concerned, there has been an increased interest in isospin-related phenomena in recent years [13]. For instance, studies of excited states of proton-rich nuclei with $N<Z$ resulted in significantly improved information on Coulomb energy differences [13]. In some cases, observed Coulomb shifts turned out to be surprisingly large [14], thus fueling speculations of significant nuclear charge-symmetry-breaking forces.

A precise description of Coulomb effects in nuclei constitutes a notoriously difficult computational challenge. In the shell-model approach to the isospin mixing (see, e.g., Refs. [13, 14]), the effective shell-model Hamiltonian including the Coulomb interaction is diagonalized in a proton-neutron basis to account for non-perturbative effects. The overall strength of the isospin-breaking interactions is usually renormalized by reproducing the rms proton point radii obtained from spherical Hartree-Fock (HF) calculations [15] or by fitting the experimental isobaric mass shifts [15, 16]. To take into account the coupling to the giant monopole resonance that appreciably influences the radial mismatch between the proton and neutron wave functions [5], single-particle wave functions can be taken from HF calculations. More precise treatments require determining the effective Coulomb inter-
action in the large space, which is possible in the no-core shell model. Such calculations have been carried out for $^{10}\text{C}$ [18] in the space allowing all $8\hbar\Omega$ excitations relative to the unperturbed ground state. Currently, however, ab-initio approaches to superallowed Fermi transitions do not go beyond $^{10}\text{C}$ which marks the state of the art.

In heavier nuclei, especially those involving many nucleons outside closed shells, the isospin mixing can be well described by the mean-field (MF) or energy-density-functional (EDF) methods [19], where the Coulomb force amounts to making the neutron and proton single-particle orbitals different, and the long-range polarization effects (e.g., those related to the isoscalar and isovector monopole resonance) are fully taken into account.

The fact that the MF methods allow for precise treatment of long-range operators is, in fact, essential for the physics of isospin mixing. However, it was very early realized [21][22][23][24] that these nice physical properties of the MF methods are accompanied by unwanted spurious effects related to the fact that the neutron and proton single-particle states in $N \neq Z$ nuclei are different even without Coulomb interaction included. Indeed, the presence of the neutron or proton excess automatically yields isovector mean fields, i.e., different HF potentials for protons and neutrons. This unwelcome feature has hampered MF calculations of the isospin mixing beyond the $N = Z$ systems (see, e.g., Ref. [23]). To overcome this difficulty in the present study, we employ the mean-field methods in the framework of Refs. [22][23], which is entirely free of the spurious isospin mixing. Thereby, for the first time, we determine the isospin mixing within the context of modern EDF methods.

We begin by noting that the self-consistent MF state $|\text{MF}\rangle$ can be expanded in good-isospin basis $|T, T_z\rangle$: 

$$
|\text{MF}\rangle = \sum_{T \geq |T_z|} b_{T, T_z} |T, T_z\rangle, \quad \sum_{T \geq |T_z|} |b_{T, T_z}|^2 = 1,
$$

where $T$ and $T_z = (N - Z)/2$ are the total isospin and its third component, respectively. The basic assumption behind our approach is that the states $|T, T_z\rangle$ capture the right balance between strong and Coulomb interactions; i.e., they contain self-consistent polarization effects to all orders. Below we shall validate this assumption by varying the MF charge $e_{\text{MF}}$, which defines the strength of the Coulomb interaction at the MF level, that is, when solving the self-consistent HF equations. On the other hand, the mixing coefficients $b_{T, T_z}$ are not reliably determined by the MF method, because they are affected by the neutron-excess-induced spurious isospin mixing.

To assess the true isospin mixing, the total Hamiltonian $\hat{H}$ (strong interaction plus the Coulomb interaction with the physical charge $e$) is rediagonalized in the space spanned by the good-isospin wave functions:

$$
|n, T_z\rangle = \sum_{T \geq |T_z|} a_{T, T_z}^n |T, T_z\rangle,
$$

where $n$ enumerates the eigenstates $|n, T_z\rangle$ of $\hat{H}$. The value of $n = 1$, corresponds to the isospin-mixed ground state (g.s.). In the following, the g.s. isospin-mixing parameter $\alpha_C = 1 - |a_{T=1, T_z}|^2$ and energy $E_{n=1, T_z}$ obtained after rediagonalization (AR) are distinguished from the quantities $\alpha_C = 1 - |b_{T=1, T_z}|^2$ and $E_{T=1, T_z} = \langle T=|T_z, T_z|\hat{H}|T=|T_z, T_z\rangle$, obtained before rediagonalization (BR; isospin projection after variation). The AR results are superior to the BR results as they are based on the double variational principle.

Our self-consistent calculations have been carried out by using the SLy4 EDF parameterization [26] and the HF solver HFODD [27] that allows for arbitrary spatial deformations of intrinsic states. Both direct and exchange Coulomb terms are calculated exactly. We adopted the standard technique of isospin projection [28]. Details pertaining to our method can be found in Ref. [29], together with numerical tests.

To illustrate the effect of the spurious isospin mixing, in Fig. 1 we show the BR and AR results for the even-even Ca isotopes. Without Coulomb interaction ($e_{\text{MF}} = 0$), there is no isospin mixing in the $N=Z$ nucleus $^{40}\text{Ca}$, but the neutron-excess-induced mixing appears in all systems with $N \neq Z$. The BR spurious mixing is quite large, $\alpha_C \approx 0.2–0.4\%$. With the the standard Coulomb interaction ($e_{\text{MF}} = e$), the BR isospin mixing increases to about 0.2–0.7\%

The AR results are entirely different. In $^{40}\text{Ca}$, with $e_{\text{MF}} = e$ we obtain the isospin mixing of 0.9\%, which is about 50\% larger than the BR value. A similar increase is predicted for other $N=Z$ systems (see the upper panel of Fig. 2). This result nicely illustrates the non-perturbative character of the Coulomb polarization when it comes to the isospin mixing. The impact of the isospin mixing on
and then decreases exponentially to about 0.01% in the g.s. structure of \( N=Z \) nuclei also shows up for the total binding energy (see the lower panel of Fig. 2). Differences between the BR and AR energies rapidly increase with mass number, to attain about 2 MeV in \( A=100 \). Interestingly, the AR values are amazingly close to the HF energies, up to 90 keV. This is a typical effect of the variational method: the minimum of energy is reasonably reproduced even if the trial wave function is rather incorrect in its detailed structure.

The AR isospin mixing is rapidly quenched with \( |N-Z| \). Indeed, \( \alpha_C \) in a \( T_z=1 \) nucleus \( ^{42}\text{Ca} \) drops to 0.2%, and then decreases exponentially to about 0.01% in \( ^{60}\text{Ca} \). As seen in Fig. 3, this behavior holds for all isotopes. It is interesting to see in Fig. 1 that the AR results obtained for \( e_{\text{MF}}=0 \) and \( e_{\text{MF}}=e \) are quite similar beyond \( ^{44}\text{Ca} \). This indicates that the correct good-isospin basis \( |T,T_z\rangle \) is generated from isospin-broken HF states even without the Coulomb interaction included on a MF level.

This fact is further corroborated by the AR results, shown in Fig. 4 relative to those obtained with the full Coulomb term, as a function of \( e_{\text{MF}} \). For \( 0.2e \leq e_{\text{MF}} \leq e \), the isospin mixing of 0.9% obtained with \( e_{\text{MF}}=e \) does not vary by more than 0.01%. At \( e_{\text{MF}}=0.2e \), the amplitude of the \( |T=2,T_z=0\rangle \) component in the MF wave function becomes too small to be included in the AR calculation; hence, the isospin mixing jumps by 0.06%. This is so, because at this small value of \( e_{\text{MF}} \), the \( \Delta T=2 \) coupling of the Coulomb force becomes ineffective and the numerical accuracy cannot be controlled. The \( |T=1,T_z=0\rangle \) component becomes very small only in the very close neighborhood of \( e_{\text{MF}}=0 \), at which point the isospin mixing disappears altogether.

The lower panel of Fig. 4 shows the total AR energy as a function of \( e_{\text{MF}} \). Here, we can understand the role of \( e_{\text{MF}} \) as a variational parameter that can be used to optimize the good-isospin basis \( |T,T_z\rangle \). It is gratifying to see that the minimum of energy is obtained almost exactly at the physical value of \( e_{\text{MF}}=e \). Namely, the optimal wave functions \( |T,T_z\rangle \) are generated by taking at the MF level the full Coulomb interaction having the physical charge. However, it is to be noted that the energy differences in Fig. 4 are quite small, of the order of a few hundred keV. Moreover, as discussed above, the isospin mixing is almost insensitive to such a refinement of \( |T,T_z\rangle \). This result supports our initial assumption: the good-isospin states \( |T,T_z\rangle \) are fairly robust to the variations of the isospin-breaking interaction, i.e., they well capture self-consistent polarization effects.

Although our results give first reliable estimates of the isospin mixing within extended MF theory, the final values of \( \alpha_C \) are still quite uncertain, which is due to an imperfect determination of the nuclear EDF. This is illustrated in Fig. 5 which shows the isospin mixing calculated in BR and AR variants for a heavy \( N=Z \) nucleus \( ^{100}\text{Sn} \) for a wide selection of the Skyrme EDF parameterizations [10]. We note that \( \alpha_C \) does depend on the nuclear effective interaction: the difference between extreme AR values obtained for SkO and SkP is as large.

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**Fig. 2:** Upper panel: isospin-mixing parameter \( \alpha_C \) in even-even \( N=Z \) nuclei calculated in BR and AR variants. Lower panel: total \( E_T=0,T_z=0 \) (BR) and \( E_{n=1,T_z=0} \) (AR) energies relative to the MF (or HF) energy \( E_{\text{MF}} \).

**Fig. 3:** The AR isospin-mixing parameter \( \alpha_C \) calculated for even-even nuclei with \( 8 \leq Z \leq 50 \) and \( -2 \leq T_z \leq 5 \).

**Fig. 4:** The isospin-mixing parameter \( \Delta \alpha_C \) (upper panel) and total energy \( \Delta E \) (lower panel) in the AR method relative to the values obtained with the full Coulomb term, plotted for \( ^{40}\text{Ca} \) as a function of \( e_{\text{MF}} \).
FIG. 5: Isospin-mixing parameter $\alpha$ in $^{100}$Sn BR (upper panel) and AR (lower panel) for various Skyrme EDF parameterizations as a function of the difference between the MF proton and neutron rms radii. Straight lines, representing linear fits, are drawn to guide the eye. See Ref. [19] for details of Skyrme functionals used.

as 1.5%, which is about 30% of the value of the isospin mixing in $^{100}$Sn.

In trying to pin down those features of the EDF that would be responsible for differences in $\alpha_C$, we have attempted to find correlations between isospin mixing and various EDF characteristics [19]. We conclude that no clear correlations exist between $\alpha_C$ and those EDF parameters that are related to nuclear-matter properties. In particular, this is true for the nuclear-matter symmetry energy, the prime suspect to influence the properties of the isovector channel. We did find a very clear correlation of the BR values of $\alpha_C$ with the differences between the MF proton and neutron rms radii (see Fig. 5). This is not surprising, as the monopole polarization does impact the proton and neutron radii, and their difference. However, after the rediagonalization, the values of $\alpha_C$ show a much weaker correlation. Clearly, the precise values of the isospin mixing parameter depend on fine details of the nuclear EDF.

In conclusion, we performed the self-consistent analysis of isospin mixing within the extended mean-field approach. Our method is non-perturbative; it fully takes into account long-range polarization effects associated with the Coulomb force and neutron excess. The nuclear Hamiltonian, including the full Coulomb interaction, is diagonalized in a good-isospin basis obtained by isospin projection from self-consistent HF states. Not surprisingly, the largest isospin-breaking effects have been predicted for $N-Z=2$ nuclei, where the effects due to the neutron (proton) excess are smallest and the Coulomb force dominates the picture.

The unphysical isospin violation caused by the neutron excess is significant on the MF level: the largest effect is predicted in $|N-Z|=2$ nuclei. However, the rediagonalization procedure eliminates the spurious isospin mixing almost completely. While the optimal many-body solutions are obtained by using the double variational approach, we have demonstrated that one obtains a reasonable good-isospin basis by broadly varying the strength of the Coulomb interaction of the EDF. Finally, we investigated the dependence of isospin mixing on the self-consistent feedback between the nuclear and Coulomb terms. We found an appreciable dependence of $\alpha_C$ on the parametrization of the nuclear functional and found a rough correlation between the isospin mixing and the difference between proton and neutron rms radii. The microscopic approach described in this study will be applied to isospin symmetry-breaking corrections to super-allowed Fermi beta decays, Coulomb energy differences, and properties of analogue states.

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[1] W. Heisenberg, Z. Phys. 78, 156 (1932).
[2] E.P. Wigner, Phys. Rev. 51, 106 (1937).
[3] G.A. Miller, A.K. Opper, and E.J. Stephenson, Ann. Rev. Nucl. Part. Sci. 56, 253 (2006).
[4] R.J. Blin-Stoyle and J. Le Tourneux, Ann. of Phys. 18, 12 (1962).
[5] G.F. Bertsch and A. Mekjian, Ann. Rev. Nucl. Sci. 22, 25 (1972).
[6] Isospin in nuclear physics, ed. D.H. Wilkinson (North Holland, Amsterdam, 1969).
[7] D.D. Warner et al., Nature Physics 2, 311 (2006).
[8] C. Horowitz et al., Nucl. Phys. A611, 211 (1996).
[9] J.C. Hardy and I.S. Towner, Phys. Rev. C71, 055501 (2005); Phys. Rev. Lett. 94, 092502 (2005); arXiv:0812.1202 (2008).
[10] I.S. Towner and J.C. Hardy, Phys. Rev. C 77, 025501 (2008).
[11] G.A. Miller and A. Schwenk, Phys. Rev. C 78, 035501 (2008).
[12] M.A. Bentley and S.M. Lenzi, Prog. Part. Nucl. Phys. 59, 497 (2007).
[13] J. Ekman et al., Phys. Rev. Lett. 92, 132502 (2004).
[14] W.E. Ormand and B.A. Brown, Nucl. Phys. A 440, 274 (1985).
[15] W.E. Ormand and B.A. Brown, Phys. Rev. C 52, 2455 (1995).
[16] M.A. Bentley et al., Phys. Lett. B 451, 445 (1999).
[17] E. Caurier et al., Phys. Rev. C 66, 024314 (2002).
[18] M. Bender et al., Rev. Mod. Phys. 75, 121 (2003).
[19] C.A. Engelbrecht and R.H. Lemmer, Phys. Rev. Lett. 24, 607 (1970).
[21] D.M. Brink and J.P. Svenne, Nucl. Phys. A 154, 449 (1970).
[22] E. Caurier et al., Phys. Lett. B 96, 11 (1980); Phys. Lett. 96B, 15 (1980).
[23] E. Caurier and A. Poves, Nucl. Phys. A385, 407 (1982).
[24] N. Auerbach, Phys. Rep. 98, 273 (1983).
[25] J. Dobaczewski and I. Hamamoto, Phys. Lett. 345B, 181 (1995).
[26] E. Chabanat et al., Physica Scripta T56, 231 (1995).
[27] J. Dobaczewski and P. Olbratowski, Comput. Phys. Commun. 158, 158 (2004); J. Dobaczewski et al., Comput. Phys. Commun., to be published.
[28] P. Ring and P. Schuck, The Nuclear Many-Body Problem (Springer-Verlag, Berlin, 1980).
[29] M. Rafalski et al., Int. Jour. Mod. Phys. E, in press; arXiv:0811.1135.