Isospin Mixing in Nuclei within the Nuclear Density Functional Theory

W. Satuła,[1] J. Dobaczewski,[1,2] W. Nazarewicz,[3,4,1] and M. Rafalski[1]

[1]*Institute of Theoretical Physics, University of Warsaw, ul. Hoża 69, 00-681 Warsaw, Poland*
[2]*Department of Physics, P.O. Box 35 (YFL), FI-40014, University of Jyväskylä, Finland*
[3]*Department of Physics & Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*
[4]*Physics Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831, USA*

(Received 6 March 2009; published 1 July 2009)

We present the self-consistent, nonperturbative analysis of isospin mixing using the nuclear density functional approach and the rediagonalization of the Coulomb interaction in the good-isospin basis. 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. A rough correlation has been found between the isospin-mixing parameter and the difference of proton and neutron rms radii.

DOI: 10.1103/PhysRevLett.103.012502 PACS numbers: 21.10.Hw, 21.30.Fe, 21.60.Jz, 23.40.Hc

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 nonperturbative. 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, nonperturbative 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 $0^+ \rightarrow 0^+$ nuclear beta decays [10] 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 [7]. 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 [15], the effective shell-model Hamiltonian including the Coulomb interaction is diagonalized in a proton-neutron basis to account for nonperturbative 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 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 interaction in the large space, which is possible in the no-core shell model. Such calculations have been carried out for ^{10}C [17] 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}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 [18], 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 [19–23] that these nice physical properties of the MF methods are accompanied by unwanted spurious effects 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. [24]). To overcome this difficulty, we employ the mean-field methods in the framework of Refs. [21,22], 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 $|\mathrm{MF}\rangle$ can be expanded in good-isospin basis $|T, T_z\rangle$:

$$|\mathrm{MF}\rangle = \sum_{T \geq |T_z|} b_{T,T_z} |T, T_z\rangle, \qquad \sum_{T \geq |T_z|} |b_{T,T_z}|^2 = 1, \quad (1)$$

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_{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 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:

$$|n, T_z\rangle = \sum_{T \geq |T_z|} a^n_{T,T_z} |T, T_z\rangle, \quad (2)$$

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.). Only those states $|T, T_z\rangle$ that have tangible contributions to the MF state (1) are used for the rediagonalization. In practice, the limit of $|b_{T,T_z}|^2 > 10^{-10}$ sets the limit of $T \leq |T_z| + 5$. In the following, the g.s. isospin-mixing parameter $\alpha_C = 1 - |a^{n=1}_{|T_z|,T_z}|^2$ and energy $E_{n=1,T_z}$ obtained after rediagonalization (AR) are distinguished from the quantities $\alpha_C = 1 - |b_{|T_z|,T_z}|^2$ and $E_{|T_z|,T_z} = \langle T = |T_z|, T_z|\hat{H}|T = |T_z|, T_z\rangle$, obtained before rediagonalization (BR; isospin projection after variation).

Our self-consistent calculations have been carried out by using the SLY4 EDF parameterization [25] and the HF solver HFODD [26] that allows for arbitrary spatial deformations of intrinsic states. Both direct and exchange Coulomb terms are calculated exactly. Details pertaining to our method can be found in Ref. [27], 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 ($e_{\mathrm{MF}} = 0$), there is no isospin mixing in the $N = Z$ nucleus ^{40}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 standard Coulomb interaction ($e_{\mathrm{MF}} = e$), the BR isospin mixing increases to about 0.2%–0.7%.

The AR results are entirely different. In ^{40}Ca, with $e_{\mathrm{MF}} = e$ 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 Fig. 2). This result nicely illustrates the nonperturbative character of the Coulomb polarization when it comes to the isospin mixing. The impact of the isospin mixing on the g.s. structure of $N = Z$ nuclei also shows up for the total binding energy (see 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 E_{MF}, 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, α_C in a $T_z = 1$ nucleus ^{42}Ca drops to 0.2%, and

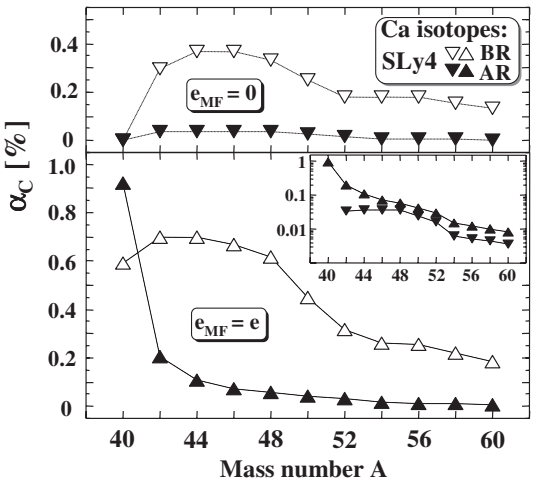

FIG. 1. Isospin-mixing parameter α_C for the even-even Ca isotopes determined before (BR) and after (AR) rediagonalization in the good-isospin basis $|T, T_z\rangle$. The basis states were generated by means of self-consistent calculations without ($e_{\mathrm{MF}} = 0$; upper panel) and with ($e_{\mathrm{MF}} = e$; lower panel) the Coulomb term. The inset shows the AR results plotted in the logarithmic scale.

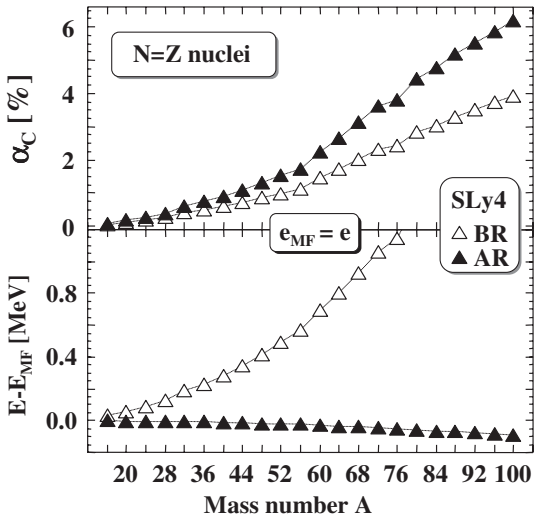

FIG. 2. Upper panel: isospin-mixing parameter α_C in even-even $N = Z$ nuclei calculated in BR and AR variants. Lower panel: total $E_{T=0,T_z=0}$ (BR) and $E_{n=1,T_z=0}$ (AR) energies relative to the MF (or HF) energy E_{MF}.

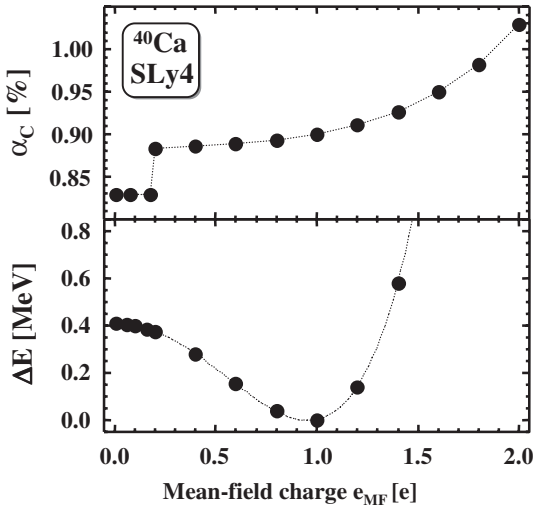

FIG. 4. The isospin-mixing parameter α_C (upper panel) and total energy ΔE relative to that obtained at $e_{\mathrm{MF}} = e$ (lower panel) plotted for ^{40}Ca as a function of e_{MF}.

then decreases exponentially to about 0.01% in ^{60}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 $e_{\mathrm{MF}} = 0$ and $e_{\mathrm{MF}} = e$ are quite similar beyond ^{44}Ca. This indicates that a good-isospin basis $|T, T_z\rangle$, which is generated from isospin-broken HF states, only weakly depends on the strength of the Coulomb interaction included on a MF level.

This fact is further corroborated by the AR results, shown in Fig. 4 as a function of e_{MF}. For $0.2e \leq e_{\mathrm{MF}} \leq e$, the isospin mixing of 0.9% obtained with $e_{\mathrm{MF}} = e$ does not vary by more than 0.01%. At $e_{\mathrm{MF}} = 0.2e$, 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_{MF}, the $\Delta T = 2$ coupling of the Coulomb force becomes ineffective and the $T = 2$ component of the MF state (1) becomes too small to be used in the rediagonalization.

The lower panel of Fig. 4 shows the total AR energy as a function of e_{MF}. Here, we can understand the role of e_{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 $e_{\mathrm{MF}} = e$. However, it is to be noted that the energy differences in Fig. 4 are quite small, of the order of a few hundred keV. These results support our initial

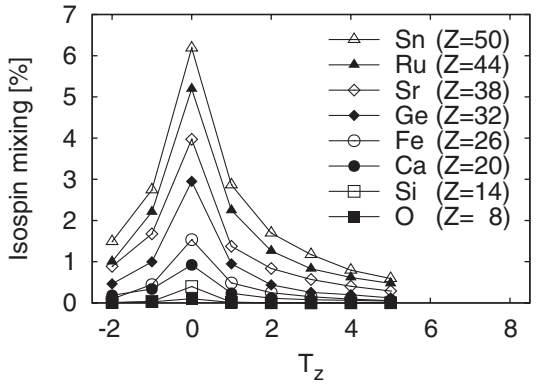

FIG. 3. The AR isospin-mixing parameter α_C calculated for even-even nuclei with $8 \leq Z \leq 50$ and $-2 \leq T_z \leq 5$.

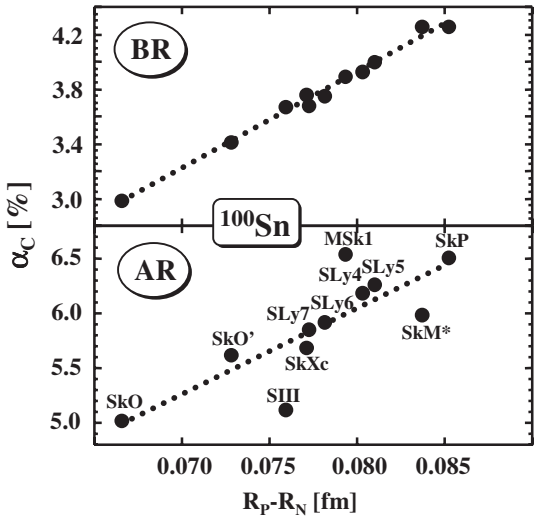

FIG. 5. Isospin-mixing parameter α_C in ^{100}Sn BR (upper panel) and AR (lower panel) for various Skyrme EDF parameterizations as a function of the difference between the MF proton and neutron rms radii. Straight lines, representing linear fits, are drawn to guide the eye. See Ref. [18] for details of the Skyrme functionals used.

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 α_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 ^{100}Sn for a wide selection of the Skyrme EDF parameterizations [18]. We note that α_C does depend on the nuclear effective interaction: the difference between extreme AR values obtained for SkO and SkP is as large 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 α_C, we have attempted to find correlations between isospin mixing and various EDF characteristics [18]. We conclude that no clear correlations exist between α_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 α_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 α_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 nonperturbative; 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. The largest isospin-breaking effects have been predicted for $N = Z$ nuclei, where the effects due to the neutron (proton) excess are smallest and the Coulomb force dominates the picture.

The unphysical isospin violation 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. 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 α_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.

Discussions with Erich Ormand are gratefully acknowledged. This work was supported in part by the Polish Ministry of Science under Contract No. N N202 328234, Academy of Finland and University of Jyväskylä within the FIDIPRO programme, and U.S. Department of Energy under Contract Nos. DE-FG02-96ER40963 (University of Tennessee) and DE-AC05-00OR22725 with UT-Battelle, LLC (Oak Ridge National Laboratory).

[1] W. Heisenberg, Z. Phys. **78**, 156 (1932).
[2] E. P. Wigner, Phys. Rev. **51**, 106 (1937).
[3] G. A. Miller *et al.*, Annu. Rev. Nucl. Part. Sci. **56**, 253 (2006).
[4] R. J. Blin-Stoyle and J. Le Tourneux, Ann. Phys. (N.Y.) **18**, 12 (1962).
[5] G. F. Bertsch and A. Mekjian, Annu. Rev. Nucl. Sci. **22**, 25 (1972).
[6] *Isospin in Nuclear Physics*, edited by D. H. Wilkinson (North Holland, Amsterdam, 1969).
[7] D. D. Warner *et al.*, Nature Phys. **2**, 311 (2006).
[8] S. Ćwiok *et al.*, Nucl. Phys. A **611**, 211 (1996).
[9] C. Horowitz *et al.*, Phys. Rev. C **72**, 035801 (2005).
[10] J. C. Hardy and I. S. Towner, Phys. Rev. C **71**, 055501 (2005); Phys. Rev. C **79**, 055502 (2009).
[11] I. S. Towner and J. C. Hardy, Phys. Rev. C **77**, 025501 (2008).
[12] G. A. Miller and A. Schwenk, Phys. Rev. C **78**, 035501 (2008).
[13] M. A. Bentley and S. M. Lenzi, Prog. Part. Nucl. Phys. **59**, 497 (2007).
[14] J. Ekman *et al.*, Phys. Rev. Lett. **92**, 132502 (2004).
[15] W. E. Ormand and B. A. Brown, Nucl. Phys. **A440**, 274 (1985); 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).
[20] D. M. Brink and J. P. Svenne, Nucl. Phys. **A154**, 449 (1970).
[21] E. Caurier *et al.*, Phys. Lett. B **96**, 11 (1980); Phys. Lett. B **96**, 15 (1980).
[22] E. Caurier and A. Poves, Nucl. Phys. **A385**, 407 (1982).
[23] N. Auerbach, Phys. Rep. **98**, 273 (1983).
[24] J. Dobaczewski and I. Hamamoto, Phys. Lett. B **345**, 181 (1995).
[25] E. Chabanat *et al.*, Phys. Scr. **T56**, 231 (1995).
[26] J. Dobaczewski and P. Olbratowski, Comput. Phys. Commun. **158**, 158 (2004).
[27] M. Rafalski *et al.*, Int. J. Mod. Phys. E **18**, 958 (2009).