RAPID COMMUNICATIONS

PHYSICAL REVIEW C VOLUME 52, NUMBER 3 SEPTEMBER 1995

Isospin mixing in proton-rich $N \simeq Z$ nuclei

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(Received 9 December 1994; revised manuscript received 7 June 1995)

Estimates of isospin mixing in proton-rich medium-heavy nuclei in the region of mass numbers $A=80$ and 100 are made with the use of Hartree-Fock (HF) calculations with Skyrme forces. An isospin mixing probability of 4–5 % is predicted in the ground state of ^{100}Sn and about 3–4 % in ^{80}Zr. These are about a factor of 2 larger than the estimates given by Bohr and Mottelson who directly evaluate the isospin mixing with a collective model description of the isovector giant monopole resonance (IVGMR). We show that if we use the energy-weighted sum rule together with the energies of the IVGMR given by Bohr and Mottelson, the predicted isospin admixtures are close to those of HF calculations. More realistic estimates of isospin mixing with random-phase approximation are also presented in the case of ^{100}Sn.

PACS number(s): 21.10.Hw, 21.60.Jz, 21.60.Ev, 27.60.+j

During recent years, with the advent of heavy-ion accelerators, it has been possible to detect and separate new proton-rich nuclei with masses ranging from 80 to 100. In particular, the identification of ^{100}Sn, predicted to be the heaviest particle-stable $N=Z$ nucleus, has been recently reported [1,2].

These nuclei, on the proton-rich side of the valley of β stability, are subject to two conflicting nuclear effects: on the one hand the attractive symmetry energy which tries to minimize the difference between neutron and proton densities, and on the other hand the repulsive Coulomb interaction. The latter is expected to dominate with increasing mass and, since this interaction does not conserve isospin, considerable isospin mixing could result in the ground state of heavy $N=Z$ nuclei. Estimates of isospin mixing have been presented recently by Hamamoto and Sagawa [3] for several exotic nuclei and their effect on the Gamow-Teller matrix element has been commented upon by Brown [4]. In the case of ^{100}Sn, Hamamoto and Sagawa [3] obtain a 4–5 % admixture of $T=1$ in the ground state, making it the largest isospin impurity in the ground state of a particle-stable even-even nucleus.

In this Rapid Communication we present calculations for the nuclei ^{80}Zr, ^{99}Sn, ^{99}In, and ^{100}Sn. In addition to ^{80}Zr and ^{100}Sn, which are two $N=Z$ nuclei of current interest, we also consider the pair of mirror nuclei ^{99}Sn and ^{99}In since these are related through superallowed Fermi transitions and, as a consequence, isospin mixing may be measurable in the β decay. In contrast to these, ^{80}Zr and ^{100}Sn can β decay only through Gamow-Teller transitions.

Hartree-Fock calculations. We first show the results of Hartree-Fock (HF) calculations with Skyrme interaction (SIII). To explore the importance of the neutron-proton interaction with regard to isospin admixtures, we present two sets of HF calculations. First, HF calculations are performed without Coulomb interaction between the protons. (This in order to check that there is no spurious isospin mixing due to the effective interaction. For $N=Z$ nuclei we obtain identical proton and neutron single-particle spectra and densities.) Next, the HF calculations are repeated with the Coulomb interaction.

To estimate isospin admixtures in the ground state we use the method suggested by Soper [5]. We assume that the part of the Coulomb force causing the isospin mixing is of isovector character. The proton single-particle wave function in the orbit (nlj), if expanded in the basis of neutron wave functions, is of the form

$$R^{\pi}_{nlj}(r)=N_{nlj}\left[R^{\nu}_{nlj}(r)+\sum_{n'\neq n}\beta^{n'}_{nlj}R^{\nu}_{n'lj}(r)\right], \tag{1}$$

where n,n' are principal quantum numbers. The Coulomb interaction has off-diagonal elements in the principal quantum number only and furthermore, the dominant contribution to the sum in Eq. (1) stems from $n'=n+1$, so that $\beta^{n'}_{nlj}=\beta^{n+1}_{nlj}$. (We shall omit the superscript $n+1$ henceforth and denote this coefficient by β_{nlj}.) The admixture of $T=T_0+1$ into the ground state with isospin T_0 is then given by [5]

$$P(T=T_0+1)=\frac{1}{2(T_0+1)}\sum_{nlj}{}' \mathcal{N}_{nlj}\beta^2_{nlj}, \tag{2}$$

where $\mathcal{N}_{nlj}$ is the number of protons in the orbit (nlj) and the prime implies that only those orbits (nlj) are included in the sum for which the neutron orbit $(n+1,lj)$ is not occupied. For small isospin admixtures one has that the deviation from unity in the overlaps of the neutron and proton wave functions,

$$C_{nlj}\equiv 1-\int_0^{\infty}R^{\pi}_{nlj}(r)R^{\nu}_{nlj}(r)r^2dr=1-N_{nlj}, \tag{3}$$

is approximately given by

$$C_{nlj}=1-\frac{1}{\sqrt{1+\beta^2_{nlj}}}\approx\frac{1}{2}\beta^2_{nlj}, \tag{4}$$

TABLE I. Values of the coefficients C_{nlj} for the different orbitals in ^{100}Sn, as resulting from an HF calculation. For the difference between the two columns, see text.

Orbit	$C_{nlj}^{(0)}$	$C_{nlj}^{(1)}$
$1s1/2$	1.4×10^{-3}	6.0×10^{-4}
$1p3/2$	1.3×10^{-3}	6.0×10^{-4}
$1p1/2$	1.2×10^{-3}	5.0×10^{-4}
$1d5/2$	1.3×10^{-3}	6.0×10^{-4}
$2s1/2$	3.7×10^{-3}	1.7×10^{-3}
$1d3/2$	1.4×10^{-3}	6.0×10^{-4}
$1f7/2$	1.5×10^{-3}	7.0×10^{-4}
$2p3/2$	5.0×10^{-3}	2.8×10^{-3}
$1f5/2$	1.5×10^{-3}	8.0×10^{-4}
$2p1/2$	4.9×10^{-3}	3.0×10^{-3}
$1g9/2$	2.0×10^{-3}	1.1×10^{-3}
$P(T=1)$	9.12%	4.25%

so that

$$P(T=T_0+1)=\frac{1}{T_0+1}\sum_{nlj}{}' \mathcal{N}_{nlj}C_{nlj}. \qquad (5)$$

One can thus evaluate the isospin admixture directly from the overlaps of neutron and proton single-particle wave functions.

Table I shows the values of C_{nlj} for the nucleus ^{100}Sn, obtained in two different ways. In the first, overlaps are calculated of proton wave functions from the full HF calculation with neutron wave functions from the HF calculations without Coulomb interaction. Deviations from unity in the overlaps are designated as $C_{nlj}^{(0)}$ and shown in column 2. (These overlaps will be similar to those where Woods-Saxon wave functions are used for the neutrons, and Woods-Saxon plus Coulomb for the protons. Strictly speaking these would differ from the Woods-Saxon overlaps because the proton wave functions have already taken into account the full n-p interaction.) In a second approach, overlaps of neutron and proton wave functions from the full HF calculation are computed and the resulting $C_{nlj}^{(1)}$ are shown in column 3. The latter procedure is the correct one, since it takes into account the full self-consistency of the HF method. It can be seen that the C_{nlj} coefficients obtained with the correct procedure are about a factor of 2 smaller. The $T=1$ admixtures in the ground state corresponding to these two approaches (9.12% and 4.25%, respectively) are also shown in the last row of Table I. The difference between the two estimates arises because of the neutron-proton interaction which minimizes the difference between the neutron and proton densities. This effect is illustrated in Fig. 1 which shows the isovector density $(\rho_p-\rho_n)$ for the two cases discussed above. The isovector density is reduced in the case of the full HF calculation. This effect is referred to as the induced isovector correction by Ormand and Brown [6].

Similar calculations with full HF were done for ^{80}Zr, ^{99}Sn, and ^{99}In. In the mirror nuclei ^{99}Sn and ^{99}In the $T=3/2$ states mix in the $T=1/2$ ground state. The results of the isospin admixtures in these nuclei are shown in Table II.

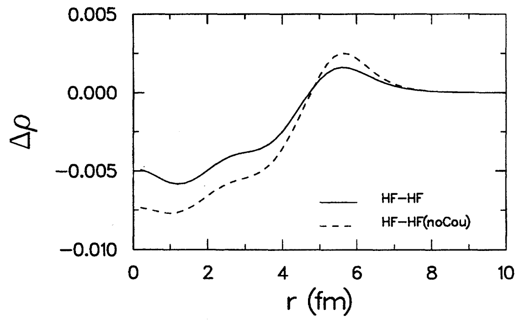

FIG. 1. Isovector density $(\rho_p-\rho_n)$ for the two cases discussed in the text. The solid line refers to the case in which both proton and neutron densities are obtained in the full HF calculation. In the case of the dashed line, the neutron density is obtained in an HF calculation without the Coulomb interaction.

These $T=3/2$ isospin admixtures in ^{99}Sn and ^{99}In are closely related to the $T=1$ admixture ^{100}Sn through the isospin factor $(T_0+1)^{-1}$.

The hybrid model. An alternative and direct means of evaluating isospin admixtures is to directly construct the $T=T_0+1$ states and evaluate Coulomb matrix elements between these and the ground state with isospin T_0. Bohr and Mottelson [7] suggested the existence of a giant isovector monopole resonance (IVGMR) which would carry most of the monopole strength. Treating the IVGMR as a compressional mode, they obtain its energy $E_{\rm IVGMR}$ as $170A^{-1/3}$ MeV. Direct evaluation [8] of the matrix element of the Coulomb interaction, described as due to a uniformly charged sphere

$$V_C=\frac{Ze^2}{2R}\left(3-\frac{r^2}{R^2}\right) \qquad (6)$$

with $R=1.24A^{1/3}$ fm, results in the isospin mixing probability

$$P(T=T_0+1)=\frac{3.50\times 10^{-7}}{T_0+1}Z^2A^{2/3}. \qquad (7)$$

This yields admixtures of 1.0% and 1.9% in ^{80}Zr and ^{100}Sn, which are about three and two times smaller, respectively, than those obtained in HF.

Alternatively, one could use a hybrid model where the isospin mixing is evaluated from the energy-weighted sum rule (EWSR) for isovector monopole excitations [9,10], i.e.,

TABLE II. Percentage admixtures of $T=T_0+1$ in the T_0 ground states of different proton-rich nuclei. The two columns refer to the predictions of HF calculations and of Eq. (11).

Nucleus	HF	Eq. (11)
^{80}Zr	3.90	2.21
^{100}Sn	4.25	4.07
^{99}In	2.77	2.48
^{99}Sn	2.83	2.59

$$\mathrm{EWSR}=\sum_{n\neq 0}(E_n-E_0)\left|\langle n|\sum_i r_i^2 t_3(i)|0\rangle\right|^2 =\frac{\hbar^2}{m}\frac{2NZ}{A}\langle r^2\rangle(1+x), \quad (8)$$

where x is the contribution from the exchange matrix elements (due to the isospin exchange part of the two-body interaction). For nuclei with masses ranging from 80 to 100, x is of the order of 0.3. The EWSR in conjunction with the energy of the IVGMR can be used to evaluate the isospin admixture $P(T=T_0+1)$, i.e.,

$$P(T=T_0+1)=\frac{1}{T_0+1}\left(\frac{Ze^2}{2R^3}\right)^2\frac{\mathrm{EWSR}}{(E_{\mathrm{IVGMR}}-E_0)^3}. \quad (9)$$

The resulting expression is

$$P(T=T_0+1)=\frac{3.28\times 10^{-6}}{T_0+1}\frac{NZ^3}{A^{4/3}}, \quad (10)$$

where use is made of $\langle r^2\rangle=\frac{3}{5}R^2$ and $R=1.2A^{1/3}$.[1] If one uses the value for E_{IVMR} as predicted by the hydrodynamical model [7], another effect must be included since neutrons and protons are subject to different average potentials resulting in a neutron-proton exchange potential of the form $\vec{t}\cdot\vec{T}$, where $\vec{t}$ is the nucleon isospin and $\vec{T}$ that of the rest of the nucleus. This potential gives rise to further increases [11] in the energy denominator by an amount $2V_1(N-Z+2)/A$ where $V_1\approx 25$ MeV and a corresponding decrease in the isospin admixture. Thus we evaluate the quantity

$$P(T=T_0+1) =\frac{16.09}{T_0+1}\frac{NZ^3}{A^{7/3}}\frac{1}{[E_{\mathrm{IVGMR}}-E_0+4V_1(T_0+1)/A]^3}. \quad (11)$$

This quantity is shown in Fig. 2 as a function of N and Z. It can be seen that the amount of isospin mixing is exceedingly small along the line of β stability. This is primarily due to the isospin factor $(T_0+1)^{-1}$ in Eq. (11), referred to by Soper [5] as the geometrical quenching, and to a lesser extent to the factor $4V_1(T_0+1)/A$ in the energy denominator (i.e., the analogue quenching). Both effects drastically quench the isospin mixing in nuclei with a neutron excess. For example, in ^{208}Pb the geometrical quenching provides a factor of 23 while the analogue quenching reduces the isospin mixing by another factor of 3. This correction should not be introduced in the formula if the energy of the monopole resonance is determined microscopically, since the isospin exchange in the nucleon-nucleon interaction is explicitly treated in this approach.

[1]Note that the quoted value of R, to be used in the rest of the paper, was used by Auerbach [9], and is different from the value used by Bohr and Mottelson. If the value of R is evaluated from the expectation value $\langle r^2\rangle$ with HF wave functions, it is usually found to be consistent with $R\approx 1.2A^{1/3}$.

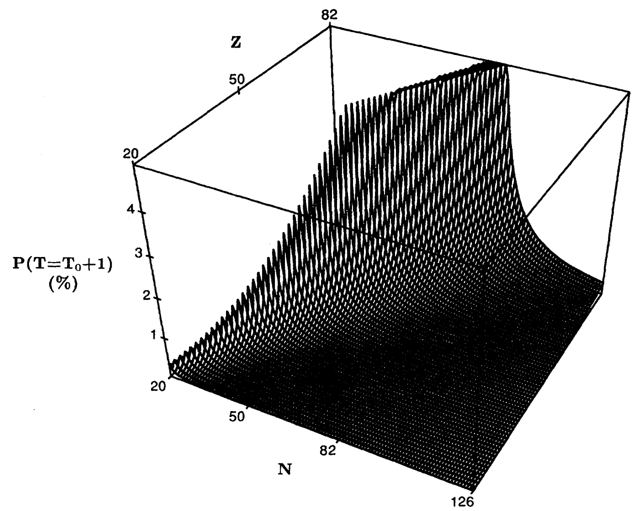

FIG. 2. Plot of the isospin mixing $P(T=T_0+1)$, Eq. (11), shown as a function of N and Z.

In Table III we compare the predictions of Eq. (11) with those of HF or RPA calculations for some of the stable nuclei [9]. Predictions of Eq. (11) for some proton-rich nuclei are shown in the third column of Table II. The expression (11) predicts admixtures comparable to those of HF in all cases except ^{80}Zr. It should be noted that HF+TDA calculations of Hamamoto and Sagawa [3] and more recent deformed HF calculations by Dobaczewski and Hamamoto [12] predict values of 3% and 2.5% for this admixture, which are much closer to the prediction of Eq. (11). All these nuclei are predicted to have similar isospin mixing in HF [except for the factor $(T_0+1)^{-1}$] because the overlaps are very similar in all cases.

The RPA calculations. To obtain a more realistic estimate, one has to go beyond HF and do RPA calculations. The results of the RPA calculations in the continuum [13] for ^{100}Sn are discussed below.

The calculation was performed with the SIII force, including in the p-h space all occupied levels, as well as up to $\Delta n=6$ unoccupied levels for each value of (l,j). This space was found to be large enough so that the RPA solutions were found to exhaust approximately 97% of the energy-weighted sum rule for the IVGMR. Following the idea of Auerbach [9] one can estimate the isospin mixing due to the Coulomb interaction by perturbation theory in the form

$$P(T=T_0+1)=\left(\frac{Ze^2}{2R^3}\right)^2\sum_{n\neq 0}\frac{|\langle n|\Sigma_i r_i^2 t_3(i)|0\rangle|^2}{(E_0-E_n)^2}, \quad (12)$$

TABLE III. Percentage admixtures of $T=T_0+1$ in the T_0 ground states of different stable nuclei. The three columns refer to the predictions of HF calculations [9], of HF+RPA [9], and of Eq. (11).

Nucleus	HF	HF+RPA	Eq. (11)
^{40}Ca	0.70	0.29	0.33
^{88}Sr	$\leq$0.5	0.17	0.19
^{208}Pb	$\leq$0.7	0.29	0.30

where $|0\rangle$ and $|n\rangle$ are the RPA ground state and excited isovector monopole states of the nucleus, with E_0 and E_n the corresponding energies. Within this perturbative approach these should be calculated by turning off the Coulomb interaction in the Hamiltonian. The resulting isospin mixing in this case was obtained as 5.2%, which should be compared with the value of about 4% predicted by the HF calculation. This increase is caused by two factors, namely, the lowering of the centroid of the isovector giant monopole resonance in RPA with respect to the empirical value $170A^{-1/3}$ predicted by Bohr and Mottelson, and more importantly due to the fact that the matrix elements of the Coulomb interaction between the RPA wave functions are considerably larger than those between the HF wave functions due to correlations. The distribution of the IVGMR predicted by RPA is shown in Fig. 3. For comparison the figure also shows the strength distribution for RPA in a discrete basis. A high dispersion of the strength of the IVGMR is apparent from the figure, together with a shift to lower energies of the centroid (at 35.9 MeV).

The RPA calculation was repeated keeping the full Coulomb interaction in the mean field. In this case one can directly evaluate the isospin mixing from the correlated ground state, with the use of the formula [9]

$$P(T=T_0+1)=0.5\langle GS|T_-T_+|GS\rangle, \tag{13}$$

where GS represents the ground state wave function. This matrix element is nothing but the m_0 sum rule (non-energy-weighted) for the operator which excites the isobaric analog state. If the GS is assumed to be the HF ground state (Tamm-Damcoff approximation), one obtains an isospin mixing of 3.8%, very close to the 4% quoted above. If instead one uses the correlated RPA ground state, Eq. (13) gives a value of 4.8% for the isospin mixing, which is close to 5.2% obtained with the perturbative approach.

In summary, HF calculations for very proton-rich nuclei in the region around $A=80$ to $A=100$ predict isospin mixing of the order of 3–5 %. The use of the EWSR in conjunction with the value of the energy of the IVGMR ($E_{\mathrm{IVGMR}}=170A^{-1/3}$) as given by Bohr and Mottelson [7] was shown to yield isospin admixtures very close to the values predicted by HF calculations. More realistic RPA calculations yield a value around 5% for isospin mixing in ^{100}Sn. An admixture of 4–5 % in probabilities imply admixtures in amplitude of around 25%. Direct tests of the isospin mixing in $N=Z$ nuclei would be through measurements of $E1$ transitions [14] or Fermi β transitions, both of which vanish in the absence of isospin mixing. Such measurements would be very useful.

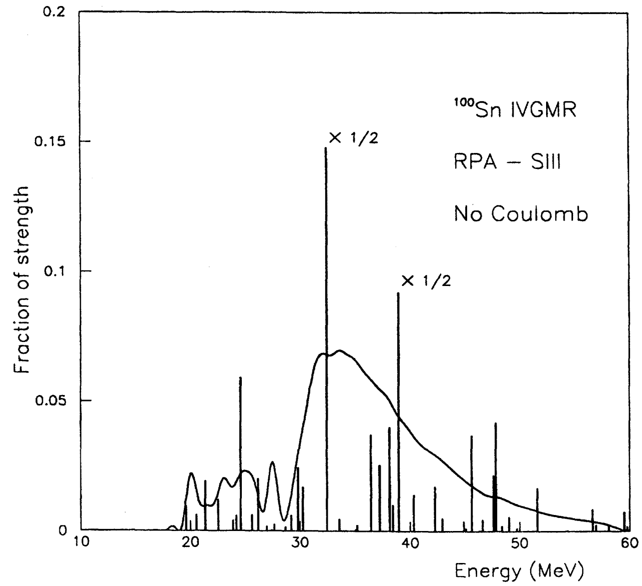

FIG. 3. RPA prediction of the distribution of the strength of the IVGMR in ^{100}Sn, shown as fraction of the sum rule. The discrete lines represent the RPA calculation in a discrete basis, while the continuous curve is the result of the RPA in the continuum. The RPA wave function used to generate the IVGMR was obtained without the Coulomb interaction in the mean field.

We would like to thank Kim Lister for bringing to our attention the observation of $E1$ transitions in ^{64}Ge [14] and Nguyen Van Giai for discussions. We gratefully acknowledge EU Contract No. CHRXCT92-0075, which in particular has allowed the stay of one of us (G.C.) in Orsay.

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