Isospin Mixing from the Effective Nucleon Interaction*

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Effective interactions determined from closed-shell-plus-two-particle spectra have a charge dependence which predicts isospin mixing for more complicated nuclei. We infer the isospin mixing in $A=44$, 46, 48, and 52 on the basis of the observed $A=42$ spectra. Agreement with experimental data is reasonable in four out of six cases; the best example is $^{48}$Sc, where we verify that the $n-p$ effective residual interaction is stronger than the $n-n$ interaction. We also compare predictions to experiment for isospin mixing in $A=20$ and 24, based on the charge dependence seen in the $A=18$ spectrum.

1. OBJECTIVES

The charge dependence of the nuclear interaction is currently under vigorous study. Not only is the subject of intrinsic interest, but recent studies of Coulomb energies of nuclei have shown that the pure Coulomb interaction, taken together with reasonable models for the nuclear wave functions, is unable to account for energy differences of mirror nuclei.1–4 The discrepancy is systematic in sign and ranges in magnitude from 100 keV in the mass-3 doublet1 to about 1 MeV in mass 208.2 In the hope of understanding the empirical charge dependence of the interaction better, we examine in this paper $\beta$-decay properties of nuclear states which are sensitive to charge dependence. In general, nuclear-structure observables which can be studied include level shifts in the spectra of isospin multiplets, and certain isospin impurities in the physical states.

Our starting point is a limited shell-model basis and an effective charge-dependent interaction determined from the simplest spectra in that basis, i.e., the one-particle and the two-particle nuclei. We apply this interaction to calculate the wave functions of heavier nuclei. Due to the charge dependence, isospin will be mixed in these heavier nuclei. This is observed experimentally by isospin-forbidden Fermi admixtures in Gamow-Teller $\beta$ decays. In the next section we discuss the interactions in our model spaces. We also briefly describe the extraction of the $\beta-\gamma$ circular polarization asymmetry, an experimentally measured quantity, from the theoretical-model wave functions. Theory and experiment are compared for nuclei in the $f_{7/2}$ shell and the $sd$ shell. We conclude that there is definite evidence in the effective interaction for a stronger $np$ force, at least in the $f_{7/2}$ shell. However, whether this is fundamental or a result of the shell truncation is unclear. In most cases, the shell description of the nuclei is not accurate enough to distinguish Coulomb from non-Coulomb sources of isospin mixing.

Previously, calculations of isospin impurities relating to isospin-forbidden $\beta$ decay were made by Blin-Stoyle and others.5–8 Our calculations are superior in the following respects: Since two-particle empirical spectra are now available, we do not have to resort to a multiparameter description of the charge-dependent interaction. Without the charge dependence as a free parameter, agreement or disagreement checks the validity of the whole shell-model approach. Also, we have better nuclear wave functions than were available previously. This is made possible by the Oak Ridge-Rochester shell-model code8 and the extensive exploration of interactions and the consequences for observables made for the $sd$-shell nuclei.

2. CHARGE-DEPENDENT INTERACTION

The evidence on the charge dependence of the nuclear force comes most fundamentally from few-body-scattering data. A comprehensive review has been given by Henley.9 One firm conclusion from the data on scattering lengths is that the neutron-proton interaction is about 2% stronger than either the neutron-neutron interaction or the non-Coulomb part of the proton-proton interaction. Unfortunately, the scattering lengths depend on the depth and range of the potential in the combination (depth)×(range)$^2$, while the properties of bound states are most sensitive to the potential depth and range in the combination (depth)×(range)$^3$. Thus an accurate measurement of the ranges of the potentials is also needed, and this is not yet available with adequate precision. The data are consistent either with an interaction having a charge-independent volume integral and/or with an interaction 2% stronger in the neutron-proton system.

To determine the charge dependence of the shell-model interaction, we turn to the spectra of nuclei that we can describe simply in the shell model.
The simplest nontrivial shell-model spectra are associated with nuclei having two valence particles of spin $j, j'$ outside of a doubly-magic core. Key states in the low-energy spectrum are interpreted as the $j \times j' = J$ couplings of the two valence particles, where the $j = j'$ situation is the simplest to treat. The $f_{7/2}$ shell has long been considered a good example; in Fig. 1 we show the spectra for the mass-42 nuclei, which we describe as two valence particles in the $f_{7/2}$ shell with a mass-40 core. The $^{40}$Ca spectrum is taken from the compilation of Endt and Van der Leun,\textsuperscript{11} the $^{42}$Sc energies are based on Ref. 12, and the $^{42}$Ti energies are based on Ref. 13.

To compare the absolute binding energies of these nuclei, we will subtract the single-particle energies of the $f_{7/2}$ nuclei. In the spirit of the shell model, these energies are just the binding-energy differences of the mass-41 nuclei. Thus the $A = 42$ spectrum plotted in Fig. 1 is determined from

$$E^{\text{nucl}}(J) = E^p(J) - E^{[40]Ca} - p [E^{[42]Sc} - E^{[42]Ca}],$$

where $p$ is the number of valence protons in the nucleus. The ground-state binding energies $E$

\begin{center}
\begin{tabular}{c|c|c|c}
$A = 42$ & ENERGIES & & \\

\hline

6$^+$ & 3.191 & -0.010 & +0.398 \\

4$^+$ & 2.750 & -0.003 & & \\

2$^+$ & 1.523 & +0.005 & & \\

0$^+$ & -0.065 & & +0.475 \\

\hline

$^{42}$Ca & $^{42}$Sc (T=I) & $^{42}$Ti & \\

\end{tabular}
\end{center}

FIG. 1. The mass-42 triad, showing the lowest $T=1$ states of each spin allowed by the coupling $f_{7/2}^2$. The energies of the different nuclei have been shifted to remove the single-particle energies with Eq. (1). Numbers above $^{42}$Ca are excitation energies in MeV, and numbers above $^{42}$Sc and $^{42}$Ti are residual shifts from the Ca energies.

used in Eq. (1) are from the compilation of Wapstra and Gove.\textsuperscript{14} We will then use in our Hamiltonian calculation the interaction matrix elements

$$\langle \frac{3}{2} \frac{3}{2} | V | \frac{3}{2} \frac{3}{2} \rangle_j = E^{\text{ex}}_j(J) + \text{constant}. \quad (2)$$

From Fig. 1 we note that the $J=0$ interaction in $^{42}$Sc is more attractive than in $^{40}$Ca, while the higher $J$ states have nearly the same interaction. This is exactly what one would expect from a short-range charge-dependent interaction stronger in $n-p$ than in $n-n$. However, the two-particle spectrum is not conclusive evidence of a fundamental charge dependence; such an effect can be obtained from the pure Coulomb interaction when the wave functions are refined.\textsuperscript{15}

Besides level shifts due to systematic Coulomb effects, there is also the possibility of particular causes, such as perturbations by nearby levels. This is bothersome in mass 42, where there are low-lying deformed states which mix substantially with the closed-shell-plus-two-particle configurations. A fit of Coulomb energies of many $f_{7/2}$ nuclei by Jänecke\textsuperscript{16} found that $^{42}$Sc was poorly fitted, being overbound by 50 keV. Jumping ahead to our conclusions, we shall find that the extra $n-p$ attraction is needed in the effective interaction of at least one other $f_{7/2}$ nucleus to account for isospin mixing.

The experimental information on $^{42}$Ti, the third member of the $A = 42$ triplet, is incomplete since the $6^+$ level is unknown. However, the systematics of the $0^+, 2^+$, and $4^+$ levels are reasonably clear. All of the levels have a large shift due to the Coulomb interaction between valence protons. In the sequel, we assume that the $6^+$ level is shifted by 10 keV less than the $4^+$. With this assumption, the average level shift is 415 keV, much larger than any theoretical calculation. Jänecke's fit of the $A = 42 f_{7/2}$ nuclei gave 330 keV for the average, which is in agreement with the theoretical Coulomb interaction in the pure $(f_{7/2})^2$ configuration. This result certainly argues against our program of using the 42 spectra to calculate properties of heavier nuclei. However, the average interaction is not relevant for isospin mixing; all that matters is the differences in level shifts. This is often parametrized by the pairing $\pi$, defined for a $j$ shell as

$$\pi_j = \frac{2j}{2j-1} (V_j - \overline{V});$$

$$\overline{V} = \sum_{J=0}^{2j-1} V_j (2j+1) \sum_{J=0}^{2j-1} (2J+1). \quad (3)$$

The $^{42}$Ti empirical spectrum has $\pi = 70$ keV, in agreement with Jänecke's results.

We will also consider nuclei in the lower $sd$
shell, where the shell model has also been successful. The empirical charge-dependent interaction is to be based on the spectra of the mass-18 triad, which is shown in Fig. 2. The data in this figure are from the compilations of Refs. 14 and 17. Similarities to the mass-42 triad may be noted. The n-p 0⁺ is anomalously low; Coulomb pairing is evident in the p-p level shifts. We shall describe these levels with the space of the full major shell, d₃/₂, s₁/₂, and d₅/₂, since this large space is necessary for a reasonable account of the properties of heavier sd nuclei.¹⁸ There is too much freedom in the Hamiltonian to use the empirical treatment for the full interaction, so we start with a nuclear interaction similar to (K + 12FP) of Ref. 18, and allow charge dependence only through the empirical one-body Hamiltonian and the Coulomb perturbation on the two-body Hamiltonian.

The one-body Hamiltonian from the mass-17 spectrum has the well-known Thomas–Ehrenmann shift of the s₁/₂ single-particle energy, amounting to 370 keV. The 0⁺ in mass 18 has a substantial admixture of the s₁/₂ configuration (23%), giving a one-body shift of 70 keV per proton. This compares well with the empirical 65-keV shift between ¹⁸⁷F(0⁺) and ¹⁸⁰O(0⁺).

For the Coulomb part of the interaction, we first tried the matrix elements of 〈r²/r₄〉 between oscillator states of ḷ=1⁴ MeV. These turned out to be too weak, so in the final calculations the Coulomb interactions in J = 0, 2, and 4 proton pairs were renormalized by factors of 1.28, 1.15, and 1.05, respectively. The resulting Hamiltonian reproduces level shifts in the A=18 triad to within 5 keV, with the exception of the 2⁺ states in ¹⁸⁷F and ¹⁸⁰Ne. The calculated ¹⁸⁷F state is strongly perturbed by a nearby theoretical T=0 state, which actually lies a safe distance away in the empirical spectrum. We have no explanation for the 100-keV discrepancy in the ¹⁸⁰Ne 2⁺ state.

In the heavier sd-shell nuclei, limitations of the computer force us to truncate the shell-model space. We calculate isospin mixing in ⁴⁴Mg, but can only use the d₅/₂ and s₁/₂ shells. The d₅/₂ orbit does not play a significant role in the level shifts of A=18, so we use the same charge-dependent Hamiltonian in the two-shell calculation.

Kahana¹⁹ has made a specific calculation of charge-dependent effects in mass 18, using d₅/₂ and s₁/₂ shells as well as core-excited configurations to describe the states. Also, he allows the single-particle wave functions to vary, which we would characterize as major shell mixing. He then finds that the ¹⁸⁷F is not shifted by the one-body Hamiltonian, i.e., a short-range fundamental charge dependence is necessary. His model has the same difficulty with the ¹⁸⁰Ne 2⁺ state as does ours.

3. CALCULATION OF ISOSPIN-FORBIDDEN β DECAY

With the interaction and configuration space specified, we calculate the wave functions of

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FIG. 2. The mass-18 triad, showing the lowest T=1 states of each spin allowed by the coupling d₅/₂. As in Fig. 2, we have subtracted the single-particle Coulomb energies and give the residual level shifts for ¹⁸⁷F and ¹⁸⁰Ne.

FIG. 3. Scheme of isospin mixing. In this case, the mixing of states in ⁴⁴Sc with T=2, J=2⁺ and T=1, J=2⁺ is measurable from the Fermi admixture in the β decay of the ⁴⁴Sc ground state to ⁴⁴Ca.
heavier nuclei using the Oak Ridge-Rochester shell-model codes described in Ref. 9. The wave functions were set up in a neutron-proton formalism to facilitate introduction of the charge-dependent interaction. An associated code is used to calculate the matrix elements of transition operators. The physical situation we investigate is the Fermi admixtures in allowed Gamow-Teller $\beta$ decays. A typical transition is shown in Fig. 3. The matrix elements of the Fermi operator, 
\[ \sum_i \tau_i^z = T^z, \quad \langle \tau^2 \rangle = \frac{3}{4}, \]
connect only analog states, so there is no transition strength between states of different $T$. No such selection rule applies to the Gamow-Teller operator:
\[ \sum_i \tau_i^z \tau_i^z, \quad \langle \sigma^2 \rangle = 3. \]
An admixture of a Fermi amplitude into the predominant Gamow-Teller decay, therefore, must be due to isospin mixing of the nuclear states. Experimentally, the Fermi admixture can be determined by careful observation of the circular polarization asymmetry of a subsequent $\gamma$ decay. The theory of the $\beta$-$\gamma$ asymmetry is derived in the book by Schopper.20 The matrix elements from state $J_i$ to state $J_f$ are customarily defined:
\[ M_F = \langle J_f M | T^+ | J_i M \rangle, \]
\[ M_{GT} = \sum_{J_f \mu} \langle J_f M | J_i M | \sum_i \tau_i^z \sigma^0 | J_f M \rangle. \]
(4)
The asymmetry depends only on the ratio of transition amplitudes $y$,
\[ y = \frac{C_F M_F}{C_A M_{GT}}. \]
(5)
Here $C_F/C_A = -1/1.23$ is the ratio of coupling constants for the transitions. The $\gamma$-polarization-asymmetry coefficient $A$ is then given by:
\[ A = \frac{\sqrt{3}}{6} \left\{ \frac{1}{1+y^2} \left[ \frac{J_f(J_f+1) - J_i(J_i+1) + 2}{[J_f(J_f+1)]^{1/2}} \right] + 4y \right\} \times F_1(LLJ_fJ_f). \]
(6)
In this formula the sign of the first term in braces is negative or positive depending on whether the transition is by electron or positron decay. The $\gamma$ decay is assumed to proceed by a multipolarity $L$ between the $\beta$-populated state $J_f$ and the $\gamma$-populated state $J_{\gamma}$. The geometric coefficient $F_1$ is defined by Rose and Biedenharn21 in terms of 3- and 6-J symbols as:
\[ F_1(LLJ_{\gamma}) = (-1)^{L+I_{\gamma}+1}(2L+1)(2I_{\gamma}+1)^{1/2} \times \left\{ \begin{array}{ccc} L & L & 1 \\ I_a & I_a & I_b \end{array} \right\}. \]
(7)
We have bothered to write down these standard formulas because we compare the relative phase of the Fermi and Gamow-Teller amplitudes as well as the magnitude, and need to refer to a precise definition. Phases are notoriously difficult to establish with uniform convention, but in this situation we are saved much trouble by the first term in braces in Eq. (6), which is independent of the nuclear structure. Since experiments quote $A$ as well as $y$, there can be no question of the experimental phase. To make a consistent theoretical phase, we simply require $y$ to be negative for superallowed decays at the lower end of the shells. For these transitions, like the neutron decay, $M_F > 0$ and $M_{GT} > 0$.

We will quote our results for isospin mixing in terms of the Hamiltonian matrix element mixing the states of different isospin:
\[ \langle T_\gamma | V | T_\gamma \rangle \approx (E_{T_\gamma} - E_{T_\gamma})M_F/\sqrt{2T_\gamma}, \]
(8)
as well as with the ratio $y$,
\[ y^{\text{theory}} = \frac{C_F}{C_A} \frac{M_F^{\text{theory}}}{M_{GT}^{\text{theory}}}. \]
(9)
The first way is close to the theoretical objective, which is the description of the isospin dependence of the interaction. However, the phase information is preserved when the theoretical $y$ is quoted, allowing the sign as well as the magnitude of the isospin mixing to be compared with experiment. Also, since $y$ is the ratio of two matrix elements, deficiencies of the wave function which affect $M_F$ and $M_{GT}$ in the same way will cancel out. This was noted by Blin-Stoyle and Yap7 in an early calculation of $^{54}$Na decay.

4. RESULTS

$f_{7/2}$ Shell

The nuclei in the $f_{7/2}$ shell region with measured isospin mixing are $^{44}$Sc (2$^+$ g.s.), $^{46}$Ti (4$^+$), $^{48}$Ti (6$^+$), $^{46}$V (4$^+$), $^{52}$Mn (6$^+$ g.s.), and $^{54}$Mn (2$^-$). The wave functions were generated for all these nuclei with the empirical mass-42 interaction discussed in Sec. 2. Except for the charge dependence, our calculation is identical in spirit to the $f_{7/2}$ calculation of McCullen, Bayman, and Zamick.23

As a check on the reliability of the wave functions, we quote in Table I the Gamow-Teller $\log f$ values. The experimental transition rates are slower than the calculated ones by about 2–3 for the Sc and Mn transitions. This moderate hindrance may reasonably be attributed to polarization effects involving the $f_{5/2}$
shell, which would not affect other properties. Therefore, we should have some confidence in using these wave functions. The $^{46}$V transition is off by a factor of 30, so the results of the pure $f_{1/2}$ calculation are quite doubtful in this case.

The results for the isospin mixing are reported in Table II. The theoretical Hamiltonian matrix element is in reasonable agreement with experiment for four out of six cases. Only the Ti cases are in bad disagreement; experiment shows very little mixing while the $f_{1/2}$ theory predicts substantial mixing. Of course, the agreement of the theoretical and experimental $(T_e | V | T_e)$ for $^{46}$V is fortuitous, since the allowed Gamow-Teller operator came out so poorly.

In some respects $^{44}$Sc is the most interesting of the measured nuclei. Only the $n$-$n$ and the $n$-$p$ interactions are involved, and with one valence proton the single-shell description may be quite good. The calculated Hamiltonian matrix element of 15 keV is entirely due to the extra binding of the $^{44}$Sc ground state. The agreement with experiment indicates that the anomaly in $^{44}$Sc binding is not a peculiarity of this one nucleus.

### Table II. Comparison of experimental and theoretical isospin mixing in the $f_{1/2}$ nuclei. Experimental values are from the compilation of Behrens [In Proceedings of the Conference on Angular Correlations in Nuclear Disintegrations, Delft, 1970, edited by H. van Krugten and Bob van Noojen (Rotterdam Univ. Press, Groningen-Nordhoff, The Netherlands, 1971)]. The theoretical $\gamma$ coefficients are determined from the ratio of theoretical Fermi to theoretical Gamow-Teller matrix elements, Eq. (4).

| Nuclear state | $(T_e | V | T_e)_{\text{theo.}}$ (keV) | $(T_e | V | T_e)_{\text{exp.}}$ (keV) | $\gamma_{\text{exp.}}/\gamma_{\text{theory}}$ |
|---------------|-------------------------------|-------------------------------|----------------------------------|
| $^{44}$Sc($2^+$)  | 16                           | 15                           | $+1.6$                           |
| $^{46}$Ti($4^+$)  | 15                           | 3                            | $+0.3$                           |
| $^{46}$Ti($6^+$)  | 22                           | $1 \pm 1$                    | $-0.1 \pm 0.1$                   |
| $^{44}$V($4^+$)   | 14                           | 13                           | $+5.3$                           |
| $^{52}$Mn($6^+$)  | 10                           | 17                           | $-3.2$                           |
| $^{52}$Zn($4^+$)  | 9                            | 10                           | $+1.8$                           |

### Table III. Gamow-Teller log ft values in the sd shell.

<table>
<thead>
<tr>
<th>Transition $(J, T)$</th>
<th>Theory</th>
<th>Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{29}$F($2^+, 1$) $\rightarrow$ $^{29}$Ne($2^+, 0$)</td>
<td>two shell</td>
<td>4.0</td>
</tr>
<tr>
<td></td>
<td>three shell</td>
<td>5.0</td>
</tr>
<tr>
<td>$^{24}$Na($4^+, 1$) $\rightarrow$ $^{24}$Mg($4^+, 0$)</td>
<td>two shell</td>
<td>5.3</td>
</tr>
<tr>
<td></td>
<td>6.1</td>
<td></td>
</tr>
</tbody>
</table>

### Table IV. Isospin mixing in the sd shell.

| Nucleus | $(T_e | V | T_e)_{\text{theory}}$ (keV) | $(T_e | V | T_e)_{\text{exp.}}$ (keV) | $\gamma_{\text{exp.}}/\gamma_{\text{theory}}$ |
|---------|-----------------------------------|-----------------------------------|----------------------------------|
| $^{20}$Ne($2^+$) twos Shell | 29                               | $10 \pm 25$                       | $+1.1 \pm 2$                     |
| three shell | 16                               |                                   | $+0.6 \pm 1.2$                   |
| $^{24}$Mg($4^+$) two shell | $-14$                            | 5                                | $-0.9$                           |

5. CONCLUSIONS

We started with the object of learning more about the charge dependence of the effective interaction. However, with the exception of the $^{44}$Sc transition we did not progress far in this direction. Indeed, we do find order-of-magnitude agreement for many cases, but in most cases the distinguishing of Coulomb from non-Coulomb isospin viola-
tion requires a more precise model of the wave functions. We are really not entitled to expect better agreement from the Fermi operator than is achieved with other operators, such as the Gamow-Teller operator. For some of the cases the disagreement is quite bad and we ascribe this to the inadequacy of the shell-model basis. With our present approach, such cases are likely to occur near the middle of shells.

The lesson learned is that useful information can be extracted only from carefully chosen nuclei having simple structure. The nucleus $^{48}$Sc, having only one valence proton, is excellent in that it is not as likely to have extensive configuration mixing, and there is no Coulomb interaction between valence protons to mask the isospin dependence of the $n-p$ interaction. Here we find agreement for the asymmetry using the charge-dependent empirical $f_{21}$ interaction. This could be due either to a fundamental charge dependence, or to higher-order Coulomb effects outside of our model space.

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