

SOME MODEL CALCULATIONS OF COULOMB MIXING

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Received 22 September 1969

Abstract: The nucleus ^{56}Co offers a good case for testing various mechanisms of isospin mixing. The analog state is bound making the mixing calculation easier than for isobaric analog resonances. There is, however, a direct correspondence between the mechanisms in the bound case and in the continuum case. The analog states of this nucleus are at low excitation so there is hope of making detailed model calculations of all the states involved in the mixing. For these calculations we consider the $J = 0^+$ $T = 2$ state of ^{56}Co as a simple 2p–2h shell-model state. Four possibilities are offered for a nearby $T = 1$ 0^+ state. The external mixing mechanism of continuum calculations is a second-order perturbation in this case which gives matrix elements several keV in magnitude. The internal mixing caused by the off-diagonal matrix elements of the Coulomb force has been neglected in continuum calculations, but we find that in this case it can be comparatively large, of the same order of magnitude as the other mechanisms. There is sufficient disparity between the matrix elements calculated for the different models to distinguish among the models experimentally. For ^{56}Co , experimental data can be interpreted to give a mixing of 33 keV with a nearby state. This is large enough to exclude two of the models.

1. Introduction

The question of the mechanism of mixing isobaric analog states into states of lower T has been given much theoretical attention. The situation is complicated, with several mechanisms of the same order of importance. A useful formalism for unbound analog states is given by Mekjian and MacDonald¹⁾, which we hereafter refer to as MM. They give expressions for the mixing of the analog state through the proton continuum (“external mixing”) and through the anti-analog state. These two mechanisms are of the same order of magnitude for certain nuclei. For both mechanisms, only the single-particle Coulomb field is needed to obtain the isospin mixing. A third mechanism, mixing via the off-diagonal matrix elements of the Coulomb force, is claimed to be small.

In this paper we make a detailed shell-model calculation of Coulomb mixing for a simple case, the first $T = 2$ $J = 0^+$ state of ^{56}Co . Here the analog state is bound so that it is not necessary to use difficult numerical techniques such as principle value integrations to calculate the external mixing. Instead, the wave function distortion can be found by perturbation theory or the numerical integration of the Schrödinger equation.

[†] Work supported in part by the US Atomic Energy Commission and the Higgins Scientific Trust Fund and in part by the Air Force Office of Scientific Research under Contract AF 49 (638)-1545.

Previous calculations of bound state mixing have been concerned with mixing of the analog into the ground state ¹⁰). This is relevant to finding Fermi-decay matrix elements. We are concerned with mixing into states in the vicinity of the analog state, so there is a closer relationship to the continuum calculations.

The ⁵⁶Co analog state has a simple wave function and is at a low excitation energy. In this situation we can hope to make microscopic models for the $T = 1$ state and calculate all mechanisms of mixing within the shell model. We will consider various likely possibilities among multiparticle-hole configurations for the $T = 1$ states. A surprising conclusion that emerges is that the off-diagonal Coulomb force can be as important as the other mechanisms in inducing mixing.

2. Mixing mechanisms

Because of the many mechanisms that contribute to Coulomb mixing, some care is needed in setting up the formalism. The procedure is to choose a Hamiltonian, define the states in terms of it, and then treat the residual interaction in perturbation theory. A convenient choice is the Hartree-Fock Hamiltonian of the parent nucleus. The analog state is then defined with the T -lowering operator:

$$|\psi_a\rangle = T_- |\psi(T, T_z = T)\rangle. \quad (1)$$

This definition of the analog state in terms of the parent is favored by Kerman and coworkers. MM prefer to use eigenfunctions of the residual nucleus HF Hamiltonian, which do not even approximately conserve T . Having used a Hartree-Fock Hamiltonian, the wave function will be a pure configuration. Configuration admixtures will be treated in perturbation theory, and included only to the extent that they affect the Coulomb mixing.

In second-quantized notation, we can write the analog state as

$$|\psi_a\rangle = \mathcal{N} \sum_{j,m} a_{jm}^\dagger(\pi) a_{jm}(v) |\rangle, \\ \mathcal{N}^{-2} = \sum_{jm} \langle a_{jm}^\dagger(v) a_{jm}(\pi) a_{jm}^\dagger(\pi) a_{jm}(v) \rangle. \quad (2)$$

Here the operator $a_{jm}(v)$ annihilates a neutron in the (j, m) orbit, and $a_{jm}^\dagger(\pi)$ creates a proton in the same orbit. The potential felt by the proton and neutron is different, which is one of the perturbations we will have to consider in the residual Hamiltonian. We define the normalized single-particle wave function $\phi_j(d)$ for the proton distortion caused by the Coulomb field in the nucleus with $T_z = T - 1$:

$$\phi_j(v) = \alpha \phi_j(\pi) + \beta \phi_j(d), \quad \alpha^2 + \beta^2 = 1. \quad (3)$$

Thus among the intermediate states that will have to be included in the calculation

are the proton distortion states,

$$|\psi_j(d)\rangle = \mathcal{N}_{j(d)} \sum_m a_{j(d)m}^\dagger(\pi) a_{jm}(\pi) |T_z = T-1\rangle. \quad (4)$$

Another state which plays an important intermediate role is the anti-analog state [refs. ^{1,2}]. This and other "configuration states" are defined by requiring a state orthogonal to the analog but with the same angular momentum structure:

$$|\psi_{\bar{a}}\rangle = \sum_j c_j \sum_m a_{jm}^\dagger(\pi) a_{jm}(v) |j\rangle, \quad (5)$$

with

$$\sum_j c_j \sum_m \langle a_{jm}^\dagger(v) a_{jm}(\pi) a_{jm}^\dagger(\pi) a_{jm}(v) \rangle = 0.$$

Because the angular momentum structure is the same as the analog, the central field can mix the two. In MM it is shown that this can be a more important intermediate state than the proton distortion states.

The states of lower isospin near the analog state we call compound states and write $|\psi_f\rangle$. For all the models we consider later these states are simple enough to mix directly with the analog state through the Coulomb force. The Coulomb force also mixes ψ_a with $\psi_{\bar{a}}$; the states $|\psi_f\rangle$ will mix with the anti-analog state via the off-diagonal nuclear force. To make a consistent treatment it is necessary to consider the same off-diagonal matrix elements for the nuclear force on the analog state. Thus besides the anti-analog, we also have to consider the intermediate states which are $T_>$ configurations, whose anti-analogs are the $|\psi_f\rangle$. Where they exist, we denote these by $|\psi_{\bar{f}}\rangle$.

For the matrix element between the analog and the compound states, we write the perturbation expansion,

$$\langle \psi_f | V_{\text{eff}} | \psi_a \rangle = \langle \psi_f | V_r | \psi_a \rangle + \langle \psi_f | V_r \frac{1}{E - H_0} V_r | \psi_a \rangle + \dots \quad (6)$$

The residual interaction can be written,

$$V_r = V_C + V'_n + (V_n - V_{\text{HF}}). \quad (7)$$

The first term V_C is the entire Coulomb force, and the second term is the nuclear interaction off-diagonal in the shell occupation numbers. The third term is the difference in the diagonal nuclear interaction from the Hartree-Fock interaction, defined for the parent state.

Obviously isospin conservation allows only V_C to contribute to the first term of (6). We will get a large contribution from the second term with a diagonal Coulomb interaction and an off-diagonal nuclear interaction. There are four terms which we consider in pairs:

$$\begin{aligned}
& \langle \psi_f | V \frac{1}{E - H_0} V | \psi_a \rangle \\
&= \left[\langle \psi_f | V_C | \psi_{\bar{f}} \rangle \frac{1}{E_f - E_{\bar{f}}} \langle \psi_{\bar{f}} | V'_n | \psi_a \rangle + \langle \psi_f | V'_n | \psi_{\bar{a}} \rangle \frac{1}{E_a - E_{\bar{a}}} \langle \psi_{\bar{a}} | V_C | \psi_a \rangle \right] \\
&+ \left[\langle \psi_f | V_C | \psi_{f(d)} \rangle \frac{1}{E_f - E_{f(d)}} \langle \psi_{f(d)} | V'_n | \psi_a \rangle + \langle \psi_f | V'_n | \psi_{a(d)} \rangle \frac{1}{E_a - E_{a(d)}} \langle \psi_{a(d)} | V_C | \psi_a \rangle \right].
\end{aligned} \quad (8)$$

For the first two terms, involving the anti-analogs $\psi_{\bar{f}}$ and $\psi_{\bar{a}}$ we make the approximation that the energy denominators are equal and opposite. The relative positions of the states is illustrated in fig. 1. The first two terms then reduce to $(V_C^{ff} V_n^{\bar{f}a} - V_n^{\bar{f}a} V_C^{aa}) / \Delta E$. The off-diagonal nuclear force will only contribute to this sum in the isospin combination, $V_{(T=1)} - V_{(T=0)}$. This would be apparent immediately in Kerman's commutator formalism.

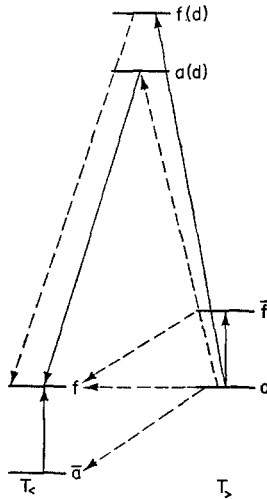


Fig. 1. Scheme of isospin mixing mechanisms. States on left are $T_<$ compound states, on right $T_>$ nuclear states. States in middle have a Coulomb-distorted single-particle wave function, with no definite isospin. In the shell-model formalism these states are shell-model excitations ≈ 15 MeV in excitation. In ref. ¹⁾ with an unbound formalism these states are degenerate with the analog.

The last two terms give the mixing via the distorted single-particle states. For isobaric analog states in the continuum, these states are degenerate with the analog, and a principal value integral is required to compute the second order mixing. This is given by MM's eq. (4.2). In our case the distorted states have a high excitation allowing the use of perturbation theory. The Coulomb part of this perturbation will be evaluated as

$$\frac{\langle \psi_{(d)} | V_C | \psi \rangle}{E - E_{(d)}} = \beta \langle \psi_{(d)} | \sum_j a_{j(d)}^\dagger(\pi) a_j(\pi) | \psi \rangle. \quad (9)$$

The coefficient β is defined in eq. (3).

The main contribution from the term $(V_n - V_{HF})$ in the residual interaction does not come until third order in perturbation theory; via a correction to the analog - anti-analog mixing. We will take this into account implicitly in calculating the analog-anti-analog mixing, by using different wave functions for proton and neutron.

3. Model wave functions

For the test calculation in ^{56}Co , we assume simple shell-model configurations. Level schemes of ^{56}Co and nearby nuclei are given in fig. 2. The analog state, lying at 3.58 MeV, is taken as the configuration

$$|\psi_a\rangle = |(f_{7/2}^{-1} f_{7/2}^{-1})_{T=1}^{J=0} (p_{3/2} p_{3/2})_{T=1}^{J=0} \rangle_{T=2}^{J=0}. \quad (10)$$

Of course other configurations are mixed into this by the residual interaction making, for example, the wave function more deformed or more like "pairing vibrations". As noted in the last section, these will be included in perturbation theory to an approximation consistent with the model for $|\psi_f\rangle$.

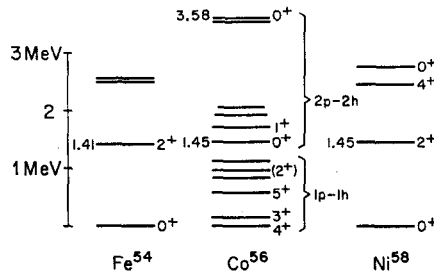


Fig. 2. The experimental levels in ^{56}Co (ref. ¹⁵). The spectrum of ^{54}Fe (ref. ⁹) and ^{58}Ni (ref. ⁴) are also given. In the shell model, ^{54}Fe is regarded as 2 holes, and ^{58}Ni as 2 particles. Then for 2p-2h states in ^{56}Co , the analog state is at 3.52 MeV excitation, and the lowest 2p-2h state, judging from the strengths in two-particle transfer reactions, is the 1.45 0^+ state. The $2^+, 3^+, 4^+, 5^+$ ground state multiplet is understood as a 1p-1h configuration.

The T -splitting of the residual interaction found from realistic interactions ³⁾ suggests that the anti-analog should be lower than the analog by a couple of MeV and indeed that there is a $J = 0$ $T = 1$ state at 1.45 MeV excitation. We write for the wave function of this state

$$|\psi_a\rangle = |(f_{7/2}^{-1} f_{7/2}^{-1})_{T=1}^{J=0} (p_{3/2} p_{3/2})_{T=1}^{J=0} \rangle_{T=1}^{J=0}. \quad (11)$$

With only two shells active, the anti-analog is the only configuration state.

It is difficult to make a reasonable model for a $T = 1$ state at the excitation of the analog. There are many possibilities, but the energetics always work out to put the state at a higher excitation.

One model that could be made from 2p-2h configurations is to recouple the angular momentum within the $p_{\frac{3}{2}}$ and $f_{\frac{7}{2}}$ configurations. A state of this kind, which we take for the first model of the compound state, is

$$|\psi_r(I)\rangle = |(f_{\frac{7}{2}}^{-2})^{J=2}_{T=1}(p_{\frac{3}{2}}^2)^{J=2}_{T=1}\rangle^{J=0}_{T=1}. \quad (12)$$

The excitation of this state relative to the anti-analog can be estimated from the excitation of the first 2^+ in ^{54}Fe and ^{58}Ni (see fig. 2). Adding the excitation of these states onto the anti-analog energy gives an excitation of 4.3 MeV for the ^{56}Co state, which is 0.7 MeV above what we require for the compound state.

A second possibility for the compound state with a 2p-2h configuration would be to have the two particles in a different shell. Diagonalizing the two-body interaction in the $p_{\frac{3}{2}}f_{\frac{7}{2}}p_{\frac{3}{2}}$ subspace gives the two lowest $J = 0$ states 4,5 separated by about 3 MeV, nearly the same as the 2.77 MeV excitation of the second 0^+ in ^{58}Ni . The mixing between shell-model configurations is quite strong, so the off-diagonal particle-particle interaction has to be included to all orders. Specifically, we take for wave functions in this, our second model,

$$\begin{aligned} |\psi_a\rangle &= |(f_{\frac{7}{2}}^{-2})^{J=0}_{T=1}(0_1^+)^{J=0}_{T=1}\rangle^{J=0}_{T=2}, \\ |\psi_r(\text{II})\rangle &= |(f_{\frac{7}{2}}^{-2})^{J=0}_{T=1}(0_2^+)^{J=0}_{T=1}\rangle^{J=0}_{T=1}, \end{aligned} \quad (13)$$

where 0_i^+ is the i th eigenstate of the ^{58}Ni Hamiltonian, $\psi_i = \sum_{jm} c_j^{(i)} a_{jm}^\dagger a_{j-m}^\dagger | \rangle$. Using the force parameters quoted in ref. ⁴), the amplitudes for the first two states in ^{58}Ni are:

	$p_{\frac{3}{2}}$	$p_{\frac{1}{2}}$	$f_{\frac{7}{2}}$
0_1^+	0.787	0.313	0.532
0_2^+	-0.600	0.188	0.778.

In this model the excitation energy of the ^{56}Co state is the anti-analog energy plus the excitation of ^{58}Ni (0_2^+). This amounts to 4.22 MeV, higher than the analog by 0.6 MeV.

Next we consider the possibility of multiparticle-hole excitations. In nuclei near the closed shells $A = 16$ and $A = 40$ multiparticle-hole states occur at quite low excitation which can be parameterized by the Bansal-French formula ⁶). If we try the same scheme regarding ^{56}Ni as the closed shell nucleus, we find different parameters for the particle-hole interaction.

Writing the monopole particle-hole force

$$V_{ph} = -a + bt_1 t_2,$$

the parameters at $A = 40$ are $a = -0.30$ and $b = 2.9$. To fit the lowest 2p-2h states in ^{56}Co , as well as the 1p-1h states, requires the parameters $a = -0.25$ and $b = 1.25$.

The T -splitting of the interaction is not as great, making it less advantageous to couple high T of particles and holes to low total T . A 3p-3h state of the configuration,

$$|\psi_{\text{f}}(\text{III})\rangle = |(f_{\frac{7}{2}}^{-3})_{T=\frac{3}{2}}^{J=\frac{3}{2}}(p_{\frac{3}{2}}^3)_{T=\frac{3}{2}}^{J=\frac{3}{2}}\rangle_{T=1}^{J=0}, \quad (14)$$

is predicted at an excitation of about 3 MeV above the analog state. We take this as our third model.

For a last model we consider the 4p-4h state

$$|\psi_{\text{f}}(\text{IV})\rangle = |(f_{\frac{7}{2}}^{-4})_{T=0}^{J=0}(p_{\frac{3}{2}}^4)_{T=0}^{J=0}\rangle_{T=1}^{J=0}. \quad (15)$$

The particle-hole interaction parameters from ^{56}Ni gives an excitation of 12 MeV for this state, while if we used the ^{40}Ca parameters, the excitation would come down to 4.5 MeV, as close to the analog as the first two models.

All the states except the third are anti-analogs of some $T = 2$ state. In other words, the compound state could have a parent in the spectrum of ^{56}Fe . Looking at the ^{56}Fe spectrum¹³), 0^+ levels are seen at 2.95, 3.60 and 4.30 MeV. The 2.95 MeV state is in accord with the $T = 2$ energies of models I and II. The problem of the energies of the $T = 1$ states is simply that the ground state anti-analog has to be shifted down 2 MeV, while the excited state anti-analog has to be shifted 3 MeV. Since the T -splitting of the lower 0^+ states is anomalously low, a larger shift for the excited 0^+ states is not unreasonable.

None of the four models above comes close in energy to the 3.52 MeV position of the observed state. But it is reasonable to hope that even though the models considered do not lie at the correct excitation, the state at that excitation will have a large amplitude of one of the model states.

4. The single-particle distortion

There are two active orbits, $f_{\frac{7}{2}}$ and $p_{\frac{3}{2}}$. The distortion of these by the Coulomb field produces an isospin mixing analogous to the external mixing of MM. The wave function can be calculated by numerically integrating the Schrödinger equation in a Woods-Saxon well. This yields[†]

$$\begin{aligned} |f_{\frac{7}{2}}(\pi)\rangle &= |f_{\frac{7}{2}}(\nu)\rangle - 0.055|f_{\frac{7}{2}}(\text{d})\rangle, \\ |2p_{\frac{3}{2}}(\pi)\rangle &= 0.995|2p_{\frac{3}{2}}(\nu)\rangle - 0.106|p_{\frac{3}{2}}(\text{d})\rangle. \end{aligned} \quad (16)$$

The single-particle wave functions are defined with the phase convention that the wave function is positive for r less than the position of the first node. Following the

[†] The author thanks Dr. W. J. Gerace for a computer program to integrate the Schrödinger equation. An accurate program is essential for finding Coulomb energy differences.

formalism of sect. 2, this can also be calculated as a perturbation. With harmonic oscillator wave function, the matrix elements of the Coulomb field are,

$$\begin{aligned}\langle 1f_{\frac{7}{2}}(i) | \sum_{j=1}^{27} V_C(ij) | 2f_{\frac{7}{2}}(i) \rangle &= +1.25 \text{ MeV}, \\ \langle 2p_{\frac{3}{2}}(i) | \sum V_C(ij) | 3p_{\frac{3}{2}}(i) \rangle &= +1.52 \text{ MeV}.\end{aligned}\quad (17)$$

In this region of the periodic table the single-particle level spacing for levels of the same spin and parity is

$$2\hbar\omega \approx 2 \times 41/A^{\frac{1}{3}} \text{ MeV} = 21 \text{ MeV}.$$

The amplitude admixture in perturbation theory is then

$$\begin{aligned}\beta_{f_{\frac{7}{2}}} &= \langle f_{\frac{7}{2}} | V_C | f'_{\frac{7}{2}} \rangle / 2\hbar\omega = -0.059, \\ \beta_{p_{\frac{3}{2}}} &= \langle p_{\frac{3}{2}} | V_C | p'_{\frac{3}{2}} \rangle / 2\hbar\omega = -0.072,\end{aligned}\quad (18)$$

to be compared with the admixtures in eq. (15). The Woods-Saxon eigenfunctions are plotted in fig. 3 along with harmonic oscillator wave functions. For the $f_{\frac{7}{2}}$, we

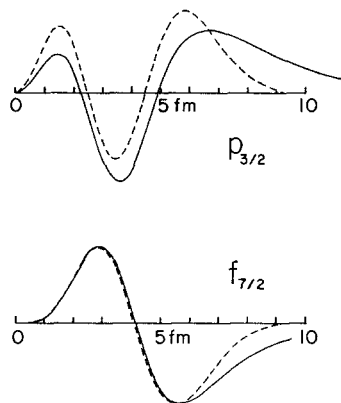


Fig. 3. The single-particle wave function distortions in ^{56}Co . The solid curve is the difference wave function between protons and neutrons; the broken curve is the harmonic oscillator state in the standard well ($\hbar\omega = 11.2 \text{ MeV}$) with one extra node.

have agreement with the Woods-Saxon result in the amplitude of the distortion as well as in the shape. The long tail of the $p_{\frac{3}{2}}$ makes the agreement poorer for p-waves. We will use the perturbation result because the nuclear matrix element and energy denominator required for eq. (8) are then easier to evaluate. The distortion found above is in agreement with other calculations along the same lines ¹⁷⁾, but is larger than the estimate in the uniform model ⁷⁾ by a factor of 2. The active orbits are concentrated on the surface, where the Coulomb field is varying more rapidly than in the interior. The uniform model gives equal weight to the interior.

5. Evaluation of matrix elements

The matrix elements V_C^{aa} and V_C^{ff} are essentially diagonal and may be expressed as the difference of single-particle Coulomb energies,

$$\langle \psi_a | V | \psi_a \rangle = \frac{1}{2} [\langle 2p_{\frac{3}{2}} | V_C | 2p_{\frac{3}{2}} \rangle - \langle 1f_{\frac{7}{2}} | V_C | 1f_{\frac{7}{2}} \rangle]. \quad (19)$$

This difference was evaluated with single-particle wave functions that are eigenstates of a Woods-Saxon well. The well was chosen to give the correct separation energy for the $p_{\frac{3}{2}}$ proton in ^{56}Co , and then the same well was used for the $f_{\frac{7}{2}}$ particle. Unfortunately the Coulomb energy difference, eq. (19) is somewhat sensitive to the choice of well. We find $\langle \psi_a | V_C | \psi_a \rangle \approx 54$ keV. Corrections to the Coulomb interaction such as the Coulomb-spin-orbit interaction, which may be of this order of magnitude (ref. ¹²), footnote 9), have been neglected. By comparison, MM found that with other shells the difference can be of the order of hundreds of keV. The result is small in this case because the $2p_{\frac{3}{2}}$ orbit is not much larger than the $f_{\frac{7}{2}}$ orbit. Experimentally, the Coulomb displacements of the $f_{\frac{7}{2}}$ shell nuclei show that the difference is small ¹⁶). Atkinson *et al.* ¹¹) assert there is a large Coulomb difference between $2p_{\frac{3}{2}}$ and $f_{\frac{7}{2}}$, but we do not find this is so with reasonable choice of well parameters.

The other matrix elements will have a rather complicated structure in terms of two-particle interactions. Fortunately, for a given model all the required matrix elements have the same angular momentum structure. The isospin structure will differ, depend-

TABLE I
Isospin structure of interaction with compound states

Model matrix element	I	II	III	IV
$\langle \psi_a V \psi_i \rangle$	$2(V_0 + V_1)$	$2(V_0 + V_1)$	$\sqrt{6}V_0 - \sqrt{2}V_1$	$\sqrt{\frac{5}{4}}V_1$
$\langle \psi_a V \psi_{\bar{i}} \rangle$	$4V_1$	$4V_1$		$\sqrt{\frac{7}{12}}V_1$
$\langle \psi_a V \psi_{f(d)} \rangle$ with particle distorted	V_1	V_1	$-\sqrt{\frac{3}{2}}V_0 + \sqrt{\frac{1}{2}}V_1$	$\sqrt{\frac{1}{20}}V_1$
hole distorted	$-V_1$	$-V_1$		$-\sqrt{\frac{1}{20}}V_1$
$\langle \psi_{a(d)} V \psi_i \rangle$ with particle distorted	V_0	V_0		
hole distorted	$-V_0$	$-V_0$	$-\sqrt{\frac{3}{2}}V_0 - \sqrt{\frac{1}{2}}V_1$	
$\langle \psi_a V \psi_f \rangle$	V_{pp}	V_{pp}	$+\sqrt{2}V_{pp}$	$\sqrt{\frac{1}{80}}V_{pp}$

Formulae are given in the text for the angular momentum reduction of matrix elements in the various models to two-body interactions. The isospin symmetry of the two-body interactions can be obtained by a similar reduction in T -space, but for convenience we tabulate the results here. V_0 and V_1 denote the two-body interaction between normalized $T = 0$ and $T = 1$ states. V_{pp} is the interaction between protons in a normalized state. In models I and II the mixing is due to a particle-hole interaction, and the isospin is in the particle-hole representation.

TABLE 2a
Two-body matrix elements for mixing calculations

Configuration	V_0	V_1	V_c
$\langle f_{\frac{1}{2}}^{-1} p_{\frac{3}{2}} V f_{\frac{1}{2}}^{-1} p_{\frac{3}{2}} \rangle_J$ $J = 2$	-1.837	1.367	-0.3125
3	-0.383	0.465	-0.3188
4	-0.617	0.211	-0.3012
5	0.626	0.470	-0.3371
$\langle f_{\frac{1}{2}}^{-1} j V f_{\frac{1}{2}}^{-1} j \rangle$ $J = \frac{3}{2}$	-0.328	+0.536	-0.3192
$\frac{1}{2}$	-0.323	+0.605	-0.3216
$\frac{5}{2}$	-0.479	+0.930	0.3237
$\langle f_{\frac{1}{2}} f_{\frac{1}{2}} V f_{\frac{1}{2}} p_{\frac{3}{2}} \rangle_J$ $J = 2$		-0.502	0.020
3	-0.482		
4		-0.307	0.022
5	-0.816		
$\langle f_{\frac{1}{2}} f_{\frac{1}{2}} V p_{\frac{3}{2}} p_{\frac{3}{2}} \rangle_0$ $J = 0$		-0.823	0.041

In this table are listed needed matrix elements which are diagonal in principal quantum numbers. The nuclear matrix elements are from Kuo ³⁾. Particle-hole matrix elements are given with J and T in particle-hole coupling. The Coulomb matrix elements were calculated explicitly using harmonic oscillator wave functions with the parameter $\hbar\omega = 11.2$ MeV. Units are MeV.

TABLE 2b
Two-body matrix elements needed for mixing calculations

Configuration	Particle distortion		Hole distortion			
	V_0	V_1	(compound)		(analog)	
			V_0	V_1	V_0	V_1
$\langle f_{\frac{1}{2}}^{-1} p_{\frac{3}{2}} V f_{\frac{1}{2}}^{-1} p_{\frac{3}{2}} \rangle$ $J = 2$	-0.038	+0.308	0.146	+0.196		
3	-0.114	+0.142	-0.070	+0.066		
4	+0.086	+0.088	0.144	+0.104		
5	+0.077	+0.079	+0.125	-0.020		
$\langle f_{\frac{1}{2}}^{-1} j V f_{\frac{1}{2}}^{-1} j \rangle$ $j = \frac{3}{2}$	+0.020	+0.131	+0.091	+0.067		
$\frac{1}{2}$	+0.050	+0.163	+0.105	+0.077		
$\frac{5}{2}$	+0.088	+0.328	-0.159	+0.251		
$\langle f_{\frac{1}{2}} f_{\frac{1}{2}} V f_{\frac{1}{2}} p_{\frac{3}{2}} \rangle$ $J = 2$		-0.012		-0.066		0.022
3	-0.093		-0.021			-0.002
4		-0.059		-0.005		0.060
5	-0.354		+0.087			-0.001
$\langle f_{\frac{1}{2}} f_{\frac{1}{2}} V p_{\frac{3}{2}} p_{\frac{3}{2}} \rangle$ $J = 0$		-0.041		0.445		

Here are given the matrix elements off-diagonal in principal quantum numbers. We list the matrix elements separately with the particle distorted and with the hole distorted. For model III the hole distortion matrix element is different for the distortion in the analog and in the compound state.

ing on whether we are considering a Coulomb or nuclear interaction. In table 1 the isospin mixtures entering the various matrix elements is tabulated. This can be derived by the same technique of angular momentum algebra used for angular recoupling.

It is useful to describe the angular recoupling in more detail, taking each model in turn. For the first model, the mixing is due to the $f_{\frac{7}{2}}-p_{\frac{3}{2}}$ particle-hole interaction, and we obtain

$$\langle \psi_a | V | \psi_f(I) \rangle = \sum_L U(\frac{7}{2} \frac{7}{2} \frac{3}{2} \frac{3}{2}; 0L) U(\frac{7}{2} \frac{7}{2} \frac{3}{2} \frac{3}{2}; 2L) \langle f_{\frac{7}{2}}^{-1} p_{\frac{3}{2}} | 2(V_0 + V_1) | f_{\frac{7}{2}}^{-1} p_{\frac{3}{2}} \rangle_L. \quad (20)$$

Similar expressions are valid for the matrix elements $\langle \psi_a | V_c | \psi_f \rangle$, $\langle \psi_a | V_n | \psi_{f(d)} \rangle$ and $\langle \psi_f | V_n | \psi_{a(d)} \rangle$, with different isospin combinations. The values of two-body matrix elements required here and below, taken mostly from the work of Kuo, are listed in table 2.

For the second model the angular structure of ψ_a and ψ_f are the same, so no Racah coefficients are needed for the matrix element. The mixing is simply given by

$$\langle \psi_a | V | \psi_f(II) \rangle = \sum_j c_j^{(1)} c_j^{(2)} \sum_L \frac{2L+1}{8(2j+1)} \langle (f_{\frac{7}{2}}^{-1} j)^L | V | (f_{\frac{7}{2}}^{-1} j)^L \rangle, \quad (21)$$

where the $c_j^{(i)}$ are the coefficients of the ^{58}Ni eigenstates defined previously. The above linear combination of interactions between the $f_{\frac{7}{2}}$ and j -shells is just the $(2L+1)$ weighed-average interaction.

TABLE 3
Coefficients of fractional parentage for calculating matrix elements to multiparticle-hole states

$\langle (p_{\frac{3}{2}}(p_{\frac{3}{2}}^2)_1^0) \frac{3}{2} \rangle p_{\frac{3}{2}}^3 \frac{3}{2} \rangle = \sqrt{\frac{5}{12}}$			
$\langle (f_{\frac{7}{2}}(f_{\frac{7}{2}}^2)_T^L) \frac{3}{2} \rangle f_{\frac{7}{2}}^3 \frac{3}{2} \rangle =$		$T = 0$	$T = 1$
$L = 2$			-0.6268
3		0.3727	
4			-0.3274
5		0.6009	
$\frac{4 \cdot 3}{2} \langle (f_{\frac{7}{2}}^2)^0 (f_{\frac{7}{2}}^2)^0 \rangle f_{\frac{7}{2}}^4 J = 0 \rangle = \sqrt{\frac{3}{2}}$			
$\frac{4 \cdot 3}{2} \langle (p_{\frac{3}{2}}^2)^0 (p_{\frac{3}{2}}^2)^0 \rangle p_{\frac{3}{2}}^4 J = 0 \rangle = 1$			

Evaluation of matrix elements for multiparticle-hole models requires coefficients of fractional parentage. We list in table 3 the needed c.f.p. In model III, where we have 3 particles coupled to $T = \frac{1}{2}$, the c.f.p. were found from orthogonality to the identical particle c.f.p., which have $T = \frac{3}{2}$. These were obtained from the appendix

of ref. ⁸). In model IV, we have wave functions of good seniority. Explicit expressions are given for the two-particle c.f.p. with seniority classification also in ref. ⁸).

In terms of the c.f.p., the matrix element for model III is

$$\begin{aligned} \langle \psi_a | V | \psi_r(\text{III}) \rangle &= \sqrt{18} \langle \{p_{\frac{1}{2}}^3\}_{\frac{1}{2}}^{\frac{1}{2}} | \{p_{\frac{1}{2}}^2\}_1^0 \}_{\frac{1}{2}}^{\frac{1}{2}} \rangle \\ &\times \sum_{L,T} \langle \{f_{\frac{1}{2}}^3\}_{\frac{1}{2}}^{\frac{1}{2}} | \{f_{\frac{1}{2}}^2\}_T^L \}_{\frac{1}{2}}^{\frac{1}{2}} \rangle \frac{1}{8} (2L+1) \langle f_{\frac{1}{2}} f_{\frac{1}{2}} | V | f_{\frac{1}{2}} p_{\frac{1}{2}} \rangle_{L,T}. \end{aligned} \quad (22)$$

The product of the c.f.p. for the model IV gives a factor $\sqrt{\frac{3}{2}}$. Except for the isospin factors, the matrix element is simply

$$\langle \psi_a | V | \psi_r(\text{IV}) \rangle = \sqrt{\frac{3}{2}} \langle p_{\frac{1}{2}} p_{\frac{1}{2}} \rangle^0 | V | (f_{\frac{1}{2}} f_{\frac{1}{2}})^0 \rangle. \quad (23)$$

The nuclear matrix elements eqs. (20)–(23) are evaluated in table 4; and the direct Coulomb matrix elements are listed in the first row of table 5. The indirect Coulomb mixing given in the next rows of table 5 is found from eq. (8), using eqs. (16)–(18) and an energy denominator for the analog state of 2.08 MeV.

TABLE 4
Matrix elements of residual nuclear interaction in ⁵⁶Co states

Model Matrix element	I (MeV)	II (MeV)	III (MeV)	IV (MeV)
$\langle \psi_a V \psi_r \rangle$	+0.592	+0.210	−1.464	−1.122
$\langle \psi_a V \psi_{\bar{r}} \rangle$	+1.192	+0.668		−0.770
$\langle \psi_{a(d)} V \psi_r \rangle$ particle distortion	−0.009	+0.030		
$\langle \psi_{a(d)} V \psi_{\bar{r}} \rangle$ hole distortion	−0.019	+0.102	−0.058	
$\langle \psi_a V \psi_{r(d)} \rangle$ particle distortion	0.042	0.083	+0.238	−0.012
$\langle \psi_a V \psi_{\bar{r}(d)} \rangle$ hole distortion	+0.004	−0.076	+0.014	−0.122

TABLE 5
Contribution of different mechanisms to Coulomb mixing in ⁵⁶Co

Model Mechanism	I (keV)	II (keV)	III (keV)	IV (keV)
direct	− 9	− 2	−18	+ 6
via anti-analogs	+12	+10	+30	+ 7
via distortion state	− 2	−10	−14	+ 8
total	+ 1	− 2	− 2	+21

6. Conclusion

We first note that all three mechanisms give contributions of roughly the same order of magnitude. It is then very important to know the phase relationship between the different mechanisms, to find the total contribution to the Coulomb mixing. From table 5 it may be seen that for the first three models there is a persistent phase relationship between the different mechanisms. The direct mixing is in phase with the second order interaction through the distortion state. This is to be expected naively from eq. (6) with a repulsive Coulomb force, an attractive nuclear force, and intermediate states higher in energy than the analog.

The mixing through the anti-analog tends to be out of phase. We see no obvious reason for a particular phase here; there is a cancellation between the mixing through the \bar{a} and \bar{f} states which can give a result of either sign.

From table 5 we see that the various models give quite different predictions for the mixing strength. In particular, models I and II have small contributions which cancel. In model III the contributions are much larger but the cancellation complete. With the disparity in the predictions of the different models, there is some hope of distinguishing between the models from the experimental data. This would be very nice because the levels higher than a few MeV are not at all well understood, as was seen from our energy estimates in sect. 3.

Recent experiments with the reactions $^{56}\text{Fe}(^3\text{He}, t)^{56}\text{Co}$ and $^{54}\text{Fe}(^3\text{He}, p)^{56}\text{Co}$ show two peaks at 3.521 and 3.587 MeV. The $(^3\text{He}, t)$ reaction [ref. ¹⁴)] shows a similar angular distribution to the two states, with strengths split in the ratio 1:2. The $(^3\text{He}, p)$ reaction ¹⁵⁾ is consistent with this. These two reactions work quite differently. Having the angular distributions the same and the ratio not changing from one reaction to the other is reasonably good evidence that the analog state is mixing with a $T = 1 \ J = 0^+$ state. Assuming that the reaction mechanism just populates the analog state, the positions of the states and the strength splittings requires a mixing of 33 keV between the pure T states.

None of the models we calculate has a mixing this large. However, there are many uncertainties in the two-body nuclear matrix elements, as well as the single-particle wave functions. In particular, we do not yet know how to calculate the off-diagonal matrix elements of the nuclear force so as to satisfy Hartree-Fock condition. The mixing via the anti-analog, proportional to the difference in Coulomb energies between $f_{\frac{3}{2}}$ and $p_{\frac{3}{2}}$, is sensitive to the details of the single-particle wave functions and other things which make the contribution from this mechanism rather uncertain.

Also, we have not discussed the isospin-violating nuclear force. According to Henley, this can be of the order of 4 % of the isospin-independent nuclear force in the singlet S-state ¹⁸⁾. From table 2a, it can be seen that this is just the same order of magnitude as the off-diagonal Coulomb force needed for model IV.

In view of these uncertainties, we would conclude that the first two models definitely have too weak mixing. Model III is not ruled out, since it does give strong mixing for

the individual contributions. Model IV is the only one, however, that gives actual order-of-magnitude agreement with experiment.

The author thanks Rubby Sherr for much advice and encouragement. Discussions of the experimental data with T. Dzubay are gratefully acknowledged.

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