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Structure of A = 53–58 Fe isotopes*

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Calculated energy levels arising from specific particle-hole configurations relative to ^{56}Ni are in good agreement with the observed spectra of A = 53–58 Fe isotopes. The energies of intruder states are closely reproduced, and spin assignments can be proposed for several known high-spin states. The energies of yrast levels, which to date have not been isolated, are predicted.

[NUCLEAR STRUCTURE ^{53,54,55,56,57,58}Fe; calculated levels, deduced particle-hole structure. Shell model with fitted effective interaction.]

I. INTRODUCTION

The large computer programs developed within the last few years have allowed shell-model calculations in the full $2s1d$-shell space for all A = 17–39 nuclei. Even with these programs, however, it is not feasible to perform calculations in the full $1f2p$-shell space for nuclei of mass much greater than 40, and rather drastic truncation must be used. Several calculations, such as the work of Horie and Ogawa[1] on $N=29$ and $N=30$ nuclei, have shown that useful results can be obtained for nuclei in the mass 50–56 region by considering only the lowest $(p_{3/2}f_{5/2}p_{1/2})^{n_p}f_{7/2}^{-n_h}$ configuration. (Here, and below, the term "configuration" refers to a specific number of particles n_p in the $p_{3/2}$, $f_{5/2}$, and $p_{1/2}$ orbitals, and a specific number of holes n_h in the $f_{7/2}$ orbital, relative to the closed-shell state of ^{56}Ni). These calculations depend for their success on the use of a suitable effective interaction which as far as possible takes into account the perturbing effects of states belonging to other configurations. In principle, these effective interactions can be obtained from a bare interaction by calculating appropriate renormalizations, but the most successful approach is to determine matrix elements by least-squares fits to selected empirical data.

Calculations which take into account the effects of one or two excited configurations by explicitly including them in the diagonalization space can be useful in giving information on the amount of configuration mixing to be expected in the lowest levels, but are of very limited use in predicting the excitation energies of levels which arise predominantly from those excited configurations. This is because the effects on these of still higher configurations are not considered, and the use of an effective interaction which attempted to do this implicitly would necessarily cause double counting in the energy shifts to the lowest configuration. Calculations of this type have typically had to use anomalously low values for the $p_{3/2}$-$f_{7/2}$ single-particle gap in order to get states from excited configurations to lie sufficiently low in the theoretical spectra. A further complication with mixed configuration calculations is that they require knowledge of many more two-body matrix elements (195, versus 111 for calculations using a single configuration). Various interactions which have been used in the $1f2p$ shell (Kuo-Brown, modified surface δ interaction, etc.) give quite different values for many of these additional matrix elements, and therefore lead to widely differing predictions for the degree of configuration mixing. It is virtually impossible to determine the matrix element by fits to empirical data.

These considerations, and the evidence from experiment that many nuclei close to ^{56}Ni have states of rather pure configurational structure (cf. for example the discussion of ^{54}Mn in Ref. 2), suggest that if a primary object of the calculations is to account for the energies of states belonging to excited configurations it is a reasonable approach to determine the spectra arising from specific values of n_p and n_h using an appropriate effective interaction. We have shown in a recent letter[2] that this type of calculation is very successful in reproducing the excitation energies of "intruder" states in mass 53–57 nuclei. The interaction, details of which are given in Ref. 2, can be divided conveniently into four parts: (i) the $f_{7/2}{}^2$ energies and $f_{7/2}$ single-hole energies, determined by a least-squares fit to 123 levels of mass 48–55 nuclei assuming pure $f_{7/2}$ configurations, (ii) the neutron-proton particle-hole interaction, determined by a least-squares fit to 63 levels of $N=29$ nuclei assuming $n_p=1$ configurations, (iii) the particle interaction, taken to be the ASDI matrix elements and single-particle energies of Koops and Glaudemans[3] which were determined by a fit to energy levels of Ni and Cu isotopes assuming $n_h = 0$, and (iv) the $T = 1\ \langle jf_{7/2}|v|j'f_{7/2}\rangle$ matrix elements, taken to be the renormalized matrix elements of Kuo and Brown[4] with a constant shift of +200 keV to all diagonals. This 200 keV shift was chosen to give an approximate best fit to intruder state energies, and is similar to that found necessary from other considerations by Sharma[5] and McGrory, Wildenthal, and Halbert.[6]

The spectra of all configurations with $n_p \leq 4$ and $n_h \leq 5$ have been calculated with this interaction and the methods described in Ref. 7, using empirical values for known $f_{7/2}^{-n_h}$ hole energies when $n_p \neq 0$. For many of these configurations the dimensions are still prohibitively large and truncation must be used. Our approach is to select the lowest 40 particle eigenstates and the lowest 40 hole eigenstates with isospin greater or equal to the minimum value which can contribute to the particle hole states of interest; as described in Ref. 7, this selection is performed with modified particle and hole energies to take into account the fact that the particle-hole interaction becomes less repulsive as the particle or hole isospin is increased. The diagonal energy of each particle-hole state of a particular J and T is then evaluated, and the final diagonalization performed including the lowest 100. Absolute binding energies relative to ^{56}Ni are closely reproduced for levels arising from a wide range of configurations, giving confidence that the truncation scheme is reasonable. Only in a few cases, when the truncation is especially severe, is there evidence that truncation causes the calculated binding energies to be in error by more than 200 keV.

In the present paper we give results for Fe isotopes of mass 53–58. These are of particular interest because of the occurrence of low-lying intruder states which cannot arise from the lowest configuration, and because of the recent observation of many high-spin states. Section II contains a discussion of the spectra, with emphasis on the structure and excitation energy of states from excited configurations. The energies of yrast levels which to date have not been isolated are predicted.

II. RESULTS

A. ^{53}Fe

Calculated spectra of the zero-particle, three-hole (0p3h) and 1p4h configurations of ^{53}Fe are shown in Fig. 1. The 2p5h configuration gives only one state below 4 MeV, a $\frac{5}{2}^-$ at 3.8 MeV. The lowest $f_{7/2}^{-3}$ states with $J < \frac{7}{2}$ are expected to lie

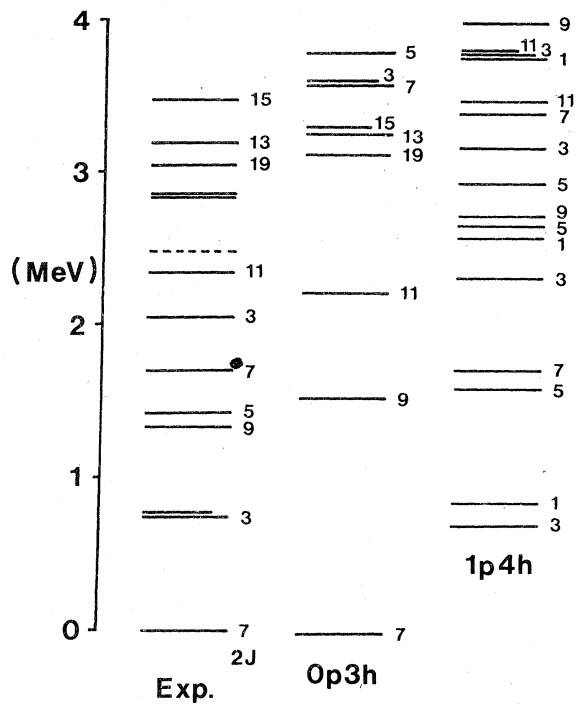

FIG. 1. The 0p3h and 1p4h spectra of ^{53}Fe.

above 3.5 MeV, and it seems clear that the only excited states below 3 MeV arising from the 0p3h configuration are the 1328 keV $\frac{9}{2}^-$ and the 2339 keV $\frac{11}{2}^-$. The $\frac{3}{2}^-$ (741 keV), $\frac{5}{2}^-$ (1423 keV), $\frac{7}{2}^-$ (1696 keV), and $\frac{3}{2}^-$ (2043 keV) levels are readily associated with 1p4h states calculated to lie at 0.69, 1.58, 1.71, and 2.31 MeV. The recently-isolated second excited state at 774 keV (Ref. 8) seems certain to be the 1p4h $\frac{1}{2}^-$ which the calculation places to 0.84 MeV. The four lowest 1p4h states are found to be over 99% neutron excitations (i.e., they have hole isospin $T_h = 0$).

States with spins greater than $\frac{19}{2}$ are predicted to lie at rather high excitation energies. The 1p4h configuration gives a $\frac{21}{2}^-$ at 7.5 MeV which is predominantly an $f_{5/2}$ particle coupled to a mixture of $T_h = 0$ and $T_h = 1$ states, and $\frac{23}{2}^-$ and $\frac{25}{2}^-$ levels at 7.6 and 8.0 MeV which are predominantly a 2p neutron coupled to the 12^+ state of ^{52}Fe. States of these spins from the 2p5h configuration lie much higher.

B. ^{54}Fe

It is clear from the results of the calculations (Fig. 2), and the high experimental level density, that the 0p2h, 1p3h, and 2p4h configurations are all important below 4 MeV. The lowest 3p5h state is calculated to be a 2^+ at 6.0 MeV. The lowest 2p4h state appears to be the 2.56 MeV 0^+, while

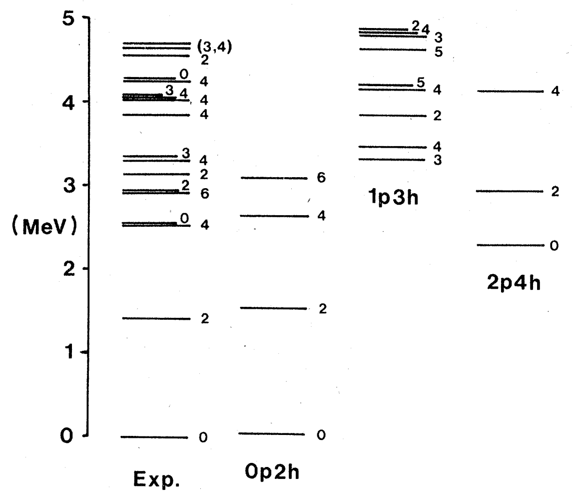

FIG. 2. The 0p2h, 1p3h, and 2p4h spectra of ^{54}Fe.

the lowest 1p3h 4^+ and 3^+ states can be associated with the levels observed at 3.30 and 3.35 MeV; these states are almost exclusively neutron excitations. Certain features of the spectrum, such as two 2^+ states in the vicinity of 3 MeV and the high density of 4^+ states close to 4 MeV, are not reproduced by the calculations. It is not clear whether this is due mainly to deficiencies of the particle-hole interaction, or to strong configuration mixing.

The 1p3h configuration gives several high-spin yrast levels between 6 and 7 MeV, with a 7^+ at 6.3 MeV and 8^+, 9^+, and 10^+ states close to 6.8 MeV. The 9^+ and 10^+ states are almost entirely a $p_{3/2}$, $f_{5/2}$, or $p_{1/2}$ neutron coupled to the $\frac{19}{2}^-$ state of ^{53}Fe, but the 7^+ and 8^+ states have more complicated structure, with large $T_h = \frac{3}{2}$ components in the 8^+. All high-spin ($J > 6$) states of the 2p4h configuration lie above 7.5 MeV. Noé *et al.*[9] have assigned probable spins of (8^+) and (10^+) to levels at 6.38 and 6.53 MeV. The (10^+) has a measured g factor of 0.78 and decays to the (8^+) with an $E2$ strength of 2 W.u. (Weisskopf unit), while with bare nucleon g factors and effective charges of $e_p = 2e$, $e_n = e$, the 1p3h calculation gives $g(10^+) = 0.65$ and $B(E2: 10 \rightarrow 8) = 1$ W.u. Noé *et al.*[9] have also isolated a level at 6.73 MeV which decays by a dipole transition to the (10^+). This is close to the calculated energy of the 9_1^+ state, but the calculated $B(M1: 9 \rightarrow 10)$ is 1.2 W.u., a factor of 18 larger than the value deduced from the measured lifetime of ~60 ps. The 10_2^+ and 11_1^+ states are calculated to lie at 7.5 and 7.8 MeV.

C. ^{55}Fe

The calculated spectrum of ^{55}Fe is in excellent agreement with experiment. Figure 3 gives the energy levels of the 1p2h and 2p3h configurations, with only high-spin states shown above 3 MeV. The 1.41 MeV level is excited strongly in neutron pick-up reactions, and is clearly to be associated with the lowest 2p3h state, which is more than 99% a neutron excitation. Sawa[10] has proposed that the 2.21 MeV ($\frac{9}{2}^-$), 2.98 MeV ($\frac{11}{2}^-$), and 3.90 MeV ($\frac{13}{2}^-$) levels constitute a band based on the neutron-hole $\frac{7}{2}^-$ state, and they should therefore be associated with the 2p3h states calculated to lie at close to the observed energies. Poletti *et al.*[11] have made spin assignments of ($\frac{19}{2}$) and ($\frac{21}{2}$) to levels at 5099 and 6529 keV; the 2p3h calculation gives yrast states of these spins at 5.2 and 6.7 MeV which are over 95% two neutrons coupled to the $\frac{19}{2}^-$ state of ^{53}Fe. Droste *et al.*[12] have observed high-spin states at 6176 and 6484 keV, with tentative spin assignments of ($\frac{21}{2}$) and ($\frac{19}{2}, \frac{21}{2}$). Since the second $\frac{21}{2}^-$ is calculated to lie at 7.6 MeV it seems likely that the 6176 keV level is actually the lowest 2p3h $\frac{17}{2}^-$, predicted at 6.1 MeV; the fact that it decays to the 2p3h $\frac{19}{2}^-$ at 5099 keV rather than to the 1p2h $\frac{15}{2}^-$ at 3419 keV can be explained by the fact that all interconfiguration transitions in ^{55}Fe appear to be greatly retarded. The 6484 keV level may be the second $\frac{19}{2}^-$ or second 2p3h $\frac{17}{2}^-$, both of which are calculated to lie at 6.6 MeV. A 1p2h $\frac{17}{2}^-$ is predicted to lie at 5.6 MeV, and the 2p3h configuration gives two closely-spaced $\frac{23}{2}^-$ states at 7.7 and 7.8 MeV.

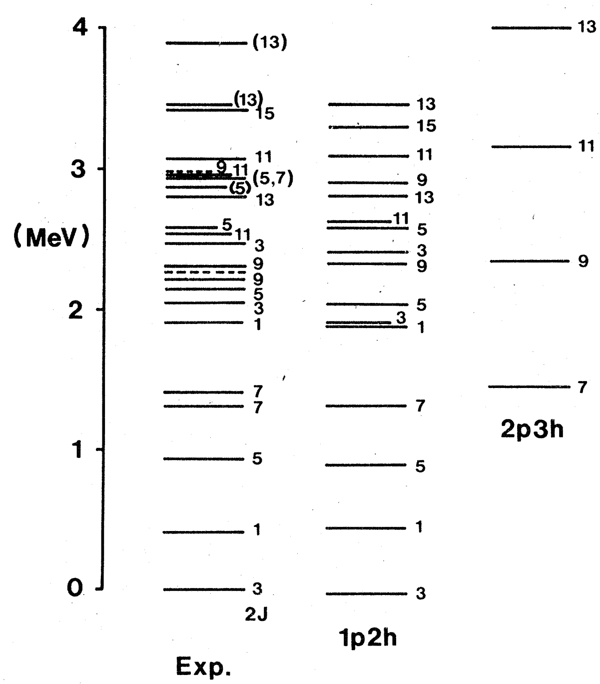

FIG. 3. The 1p2h and 2p3h spectra of ^{55}Fe. Only states with $J > \frac{9}{2}$ are shown above 3 MeV.

The lowest state arising from the 3p4h configuration is calculated to be a $\frac{1}{2}^-$ at 3.6 MeV, with $\frac{3}{2}^-$ and $\frac{5}{2}^-$ states at 3.7 and 3.75 MeV. These are found to be almost entirely two-neutron excitations with $T_p=\frac{3}{2}$, $T_h=0$, and should therefore be excited by pickup of two $f_{7/2}$ neutrons from ^{57}Fe. The $\frac{1}{2}^-$ can be associated with the 3.60 MeV level which is strongly excited by $L=0$ in the ^{57}Fe(p,t) reaction,[13] while the $\frac{3}{2}^-$ and $\frac{5}{2}^-$ states may be the $L=2$ levels observed at 3.77 and 3.89 MeV. None of these levels is excited appreciably in stripping reactions, as expected for 3p4h states.

D. ^{56}Fe

The 2p2h configuration of ^{56}Fe gives the spectrum shown in Fig. 4, and with one or two possible exceptions accounts well for all levels observed below 4 MeV. The 3p3h configuration gives nine levels between 4.1 and 5.1 MeV (two 2^+, three 3^+, three 4^+, and a 5^+), the lowest being a 2^+. Both neutron and proton excitations contribute strongly to these 3p3h states, suggesting that they may be excited both in proton stripping reactions on ^{55}Mn and in neutron pickup reactions on ^{57}Fe. Four $l=1$ levels have been observed between 4.08 and 5.2 MeV in ^{55}Mn(α,t),[14] while several strong $l=3$ levels are excited in this energy region by ^{57}Fe(d,t).[15]

Sarantites, Urbon, and Rutledge[16] and Bendjaballah *et al.*[17] have isolated the 7_1^+, 8_1^+, and 8_2^+ states of ^{56}Fe at 4701, 5255, and 5627 keV. The 2p2h calculation places these states at 4.7, 5.4, and 5.5 MeV. The level at 6116 keV may be the 8_3^+, which is calculated to lie at 6.1 MeV. The yrast 9^+ and 10^+ levels (both of 2p2h structure) are predicted to lie at 6.6 and 7.6 MeV, and 5^+ states of both 2p2h and 3p3h structure are expected close to 4.7 MeV.

The lowest two 4p4h 0^+ states are calculated to be of totally different structure, the first being of $T_p=2$, $T_h=0$ while the second is of $T_p=0$, $T_h=2$. The truncation scheme discussed in the Introduction is totally inadequate for the $T_p=2$ state, since the lowest 40 particle states include only four of $T_p=2$. A calculation using instead the lowest 40 $T_p=2$ particle states lowers the 0^+ energy from 5.3 to 4.8 MeV. The $T_h=2$ 0^+ state (calculated energy 5.7 MeV) can be associated with the 5.41 MeV level which is excited strongly by $L=0$ in the ^{54}Cr$(^3$He$,n)$ reaction.[18] This reaction also excites weakly by $L=0$ a level at 4.73 MeV which may be the predominantly $T_p=2$ state; the ^{58}Fe(p,t) reaction presumably would excite this state strongly.

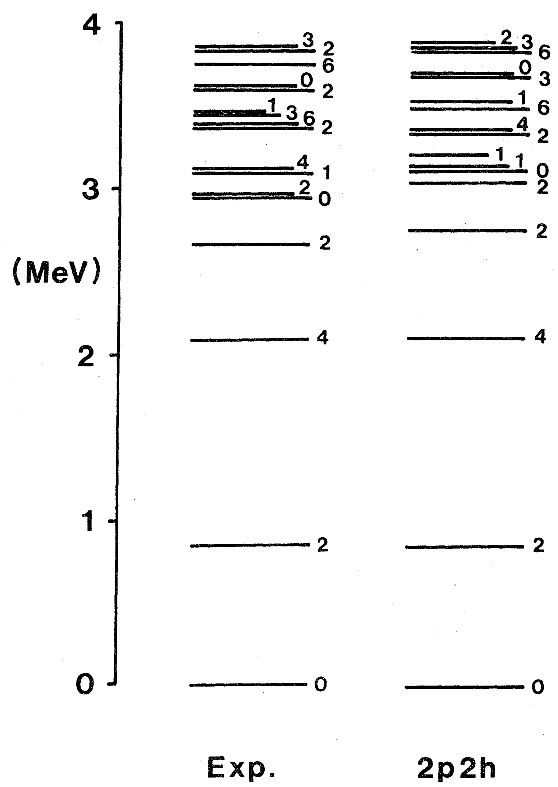

FIG. 4. The 2p2h spectrum of ^{56}Fe.

E. ^{57}Fe

The 3p2h calculation accounts satisfactorily for low-lying levels of ^{57}Fe. The spectrum is given in Fig. 5, with only high-spin states shown above 2.5 MeV, and Table I lists the calculated neutron stripping spectroscopic factors, which are in excellent agreement with experiment.[19] A large number of high-spin states are predicted to lie between 2.5 and 4 MeV. Sawa[10] has isolated three of these, and also has observed a level at 4429 keV which decays to the 3135 keV $\frac{15}{2}$ state; this is probably the lowest 3p2h $\frac{17}{2}^-$, which the calculation places at 4.5 MeV. The lowest 3p2h $\frac{19}{2}^-$, $\frac{21}{2}^-$, and $\frac{23}{2}^-$ states are predicted to lie at 5.6, 6.7, and 8.2 MeV.

The 2.22 MeV ($\frac{7}{2}^-$) level is excited strongly in the ^{58}Fe(p,d) reaction,[20] and is probably the lowest 4p3h state. A 4p3h calculation using the lowest 40 particles states of $T_p\geq 1$ (which include 9 of $T_p=2$) shows this to be an almost pure neutron-hole state, and places it at 2.8 MeV. The effects of truncation are reduced by using instead the lowest 40 $T_p=2$ particle states, the $\frac{7}{2}^-$ excitation energy then being 2.57 MeV. A further 200 keV of the discrepancy between theory and experiment is removed if empirical ^{60}Ni binding energies are used for the particles, rather than the energies given by the ASDI interaction. The only 4p3h state expected within 1 MeV of the $\frac{7}{2}^-$ is a neutron-hole

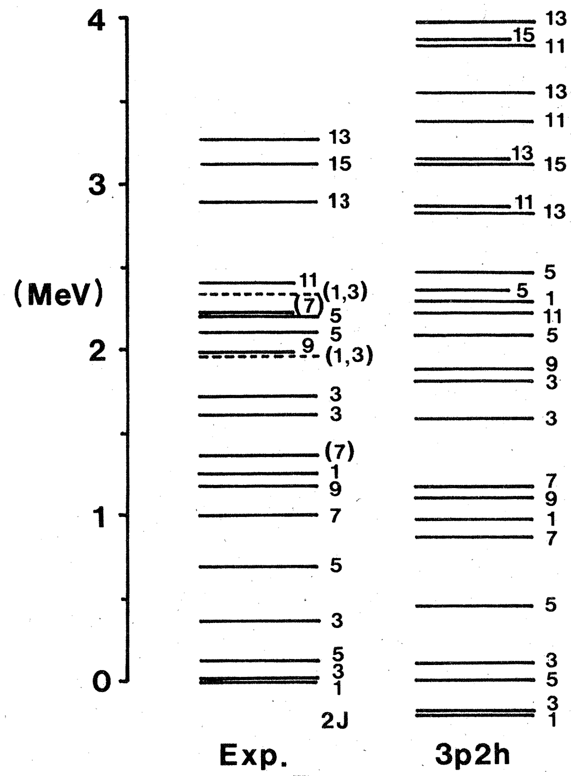

FIG. 5. The 3p2h spectrum of ^{57}Fe. Only states with $J>\frac{9}{2}$ are shown above 2.5 MeV.

$\frac{9}{2}^-$ lying 800 keV higher. The lowest $\frac{23}{2}^-$ state, which consists of various ^{60}Ni states coupled to the $\frac{19}{2}^-$ state of ^{53}Fe, is predicted to be the only yrast level below 8 MeV arising from the 4p3h configuration; it is calculated to lie a few hundred keV lower than the 3p2h state of this spin.

TABLE I. Spectroscopic factors for the ^{56}Fe$(d,p)^{57}$Fe reaction.

Level	E^* (MeV)	C^2S (expt.) (Ref. 19)	C^2S (calc.)
$\frac{1}{2}_1$	0	0.14	0.14
$\frac{3}{2}_1$	0.014	0.42	0.40
$\frac{5}{2}_1$	0.14	0.59	0.56
$\frac{3}{2}_2$	0.37	0.25	0.24
$\frac{5}{2}_2$	0.71		0.03
$\frac{1}{2}_2$	1.26	0.37	0.45
$\frac{3}{2}_3$	1.63	0.03	0.004
$\frac{3}{2}_4$	1.73	0.04	0.03
$\frac{5}{2}_3$	2.12	0.04	0.01
$\frac{5}{2}_4$	2.21	0.07	0.09

F. ^{58}Fe

The 4p2h spectrum of ^{58}Fe is shown in Fig. 6. Although the spectra of ^{58}Fe and ^{60}Ni are quite similar the calculation shows that weak coupling is an extremely poor approximation for even the low-lying states of ^{58}Fe. As is the case in ^{57}Fe, the particle-hole interaction causes strong mixing of the basis states. Writing a 4p2h state constructed by coupling the nth particle eigenvector of spin J to the hole eigenvector of spin L as $|J_n \times L\rangle$, the lowest 0^+–4^+ eigenvectors of ^{58}Fe are given by the calculation as

$$|0^+\rangle = 59\%\ |0_1\times 0\rangle + 34\%\ |2_1\times 2\rangle + \cdots,$$

$$|1^+\rangle = 41\%\ |1_1\times 0\rangle + 18\%\ |2_4\times 2\rangle + 8\%\ |3_3\times 2\rangle + 5\%\ |1_1\times 2\rangle + \cdots,$$

$$|2^+\rangle = 36\%\ |2_1\times 0\rangle + 30\%\ |0_1\times 2\rangle + 12\%\ |2_1\times 2\rangle + 7\%\ |4_2\times 2\rangle + \cdots,$$

$$|3^+\rangle = 40\%\ |3_1\times 0\rangle + 23\%\ |2_2\times 2\rangle + 12\%\ |4_1\times 2\rangle + 5\%\ |2_1\times 2\rangle + \cdots,$$

$$|4^+\rangle = 39\%\ |2_1\times 2\rangle + 23\%\ |4_2\times 0\rangle + 10\%\ |0_1\times 4\rangle + 8\%\ |4_2\times 2\rangle + \cdots,$$

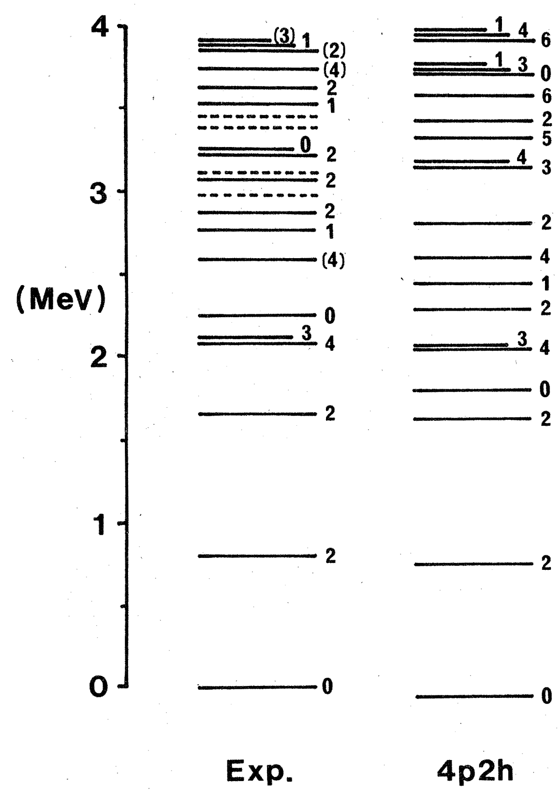

FIG. 6. The 4p2h spectrum of ^{58}Fe.

TABLE II. Spectroscopic factors for the $^{57}Fe(d,p)^{58}Fe$ reaction.

Level	C^2S (expt.) (Ref. 23)		C^2S (expt.) (Ref. 22)			C^2S (calc.)		
(keV)	$l=1$	$l=3$	$p_{1/2}$	$p_{3/2}$	$f_{5/2}$	$p_{1/2}$	$p_{3/2}$	$f_{5/2}$
$0_1(0)$	0.07		0.14			0.11		
$2_1(811)$	0.05	0.11		0.11	0.33		0.08	0.25
$2_2(1675)$	0.18	0.01		0.37			0.29	0.05
$3_1(2134)$		0.13			0.27			0.17
$0_2(2257)$	0.03					0.03		
$1_1(2782)$	0.36			0.64		0.00	0.31	
$2_3(2876)$	0.01	0.16			0.44		0.02	0.25

where only components of $\geqslant 5\%$ have been listed. Such strong mixing causes the results to be very sensitive to details of the particle eigenvectors, and therefore to the form of the particle interaction. McGrory[21] has calculated the 4p2h spectrum using a different interaction, and the excitation energies of excited 0^+ and 2^+ states differ appreciably from the present results.

The spectroscopic factors from a recent analysis of the $^{57}Fe(d,p)$ reaction[22] using polarized deuterons are much larger than values from earlier experiments[23] using unpolarized beams. The calculated values for states below 3 MeV, listed in Table II, tend to lie between the two sets of empirical numbers. The calculation successfully reproduces the $l=1$ and $l=3$ mixing in the lowest three 2^+ states, and is in agreement with experiment in giving only a very small $p_{1/2}$ strength for the lowest 1^+ state.

No high-spin states have yet been isolated in ^{58}Fe. The calculation gives yrast states of spins 7–10 at excitation energies of 5.1, 5.15, 6.15, and 7.05 MeV.

III. EXCITATION ENERGIES OF PARTICLE-HOLE STATES

It is informative to examine the various terms which contribute to the excitation energy of a particle-hole state. For example, the principal component (52%) of the 2p3h neutron-hole $\frac{7}{2}^-$ state of ^{55}Fe consists of the ground state of ^{58}Ni coupled to the ground state of ^{53}Fe. The excitation energy of this component can be expressed as

$$E^* = B(^{55}\mathrm{Fe}) + B(^{56}\mathrm{Ni}) - B(^{58}\mathrm{Ni}) - B(^{53}\mathrm{Fe}) + \langle V_{ph}\rangle ,$$

where the B are binding energies and $\langle V_{ph}\rangle$ is the particle-hole interaction energy. The binding energies sum to +210 keV and $\langle V_{ph}\rangle$ is given by the calculation as 3.3 MeV, so this component lies at an energy of 3.5 MeV. Mixing with other 2p3h states (mainly the ^{58}Ni 2_1^+ state coupled to the ground state and $\frac{9}{2}^-$ state of ^{53}Fe) depresses the energy by just over 2 MeV, leading to the observed excitation energy of 1.4 MeV.

If either the particles or holes have spin zero, an estimate of the energy of a particular weak-coupling component can readily be obtained using empirical binding energies and a simple monopole particle-hole interaction

$$V_{ph} = a + b\vec{T}_p \cdot \vec{T}_h .$$

The appropriate isoscalar and isovector strengths a and b are independent of the hole state and only weakly dependent on the particle state for two-four particles, average values with the effective interaction used being $a \approx 0.4$ MeV, $b \approx 1.8$ MeV. However, such estimates are inadequate to predict the excitation energies of actual eigenstates unless the energy reduction due to mixing of different components (which ranges up to 4 MeV in the cases considered here) can also be estimated.

IV. CONCLUSIONS

The results of these calculations show that it is possible, with a mass-independent effective interaction, to account very well for the spectra of mass 53–58 Fe isotopes making the approximation that all states arise from particular particle-hole configurations relative to ^{56}Ni. States from excited configurations can be isolated using data from particle transfer reactions, and their calculated excitation energies are in good agreement with experiment. Extreme weak coupling is found to be a very poor approximation, but in many cases over 90% of a state can be expressed in terms of only three or four components.

Calculated energies of known high-spin states in the Fe isotopes are generally in very good agreement with experiment. The predictions made concerning the energies of yrast levels which to data have not been observed should be of interest for heavy-ion reactions.

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