Theoretical Description of Energy Levels of ^{59}Fe

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The energy levels of the nucleus ^{59}Fe are described in terms of the single-particle Nilsson model. The known negative-parity levels are fitted into three rotational bands, and the location of other levels is predicted on the basis of a determination of the nuclear potential parameters. The spectroscopic factors for levels in the ground-state band are compared with the calculated values. Further checks of the model are proposed.

1. INTRODUCTION

THE experimental study of the excitation spectra of odd mass nuclei with neutron number $N=33$ has formed the subject of several investigations during the past year.[1–3] One of these nuclei, the singly closed nucleus ^{61}Ni, may reasonably be expected to have a spectrum which admits of a simple theoretical interpretation and which may in turn provide a starting point for the calculation of spectra of neighboring nuclei. Several attempts[4–7] have been made so far on the theoretical description of low-lying levels in ^{61}Ni and some of these results are presented in Fig. 1 in comparison with the experimental data. The earliest attempt was the application of the pairing plus quadrupole force model to this nucleus by Sorensen[4] and the results are shown in the second column labeled *SO* in Fig. 1. The first three states are predominantly the one-quasiparticle states, the lowest being the $\frac{5}{2}^-$ level as expected from the shell-model considerations but in contradiction to the observed $\frac{3}{2}^-$ ground state. Next the theory predicts a quintuplet of $\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, and $\frac{9}{2}$ levels around 1.3-MeV excitation followed closely by a quartet of $\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$ levels arising from the coupling of the $\frac{5}{2}^-$ and $\frac{3}{2}^-$ single-quasiparticle states, respectively, to the 2^+ state of the neighboring even-even nucleus. A comparison with the experimental excitation energies shows little similarity. Further improvements in the quasiparticle-spectrum calculations were made by Gambhir *et al.*[5] first by using the modified Tamm-Dancoff approximation (*G*1 in Fig. 1) and later by using the inverse gap equation method (*G*3 in Fig. 1) in comparison with the usual Bardeen-Cooper-Schrieffer (BCS) approach (*G*2 in Fig. 1). The results presented in *G*3 are obtained by using the experimental energies of the lowest three states as the input data. The agreement with the experiment cannot be termed as entirely satisfactory for any of these approaches. Next we have listed the phenomenological shell-model approaches, one[6] using the Talmi method of determining the two-body matrix elements directly from the experimental data and the other[7] following the determination of the parameters of the effective interaction from the experimental data for Ni isotopes. In the latter study[7] it was concluded that "even after invoking strong configuration admixtures no conventional shell-model potential, even with tensor and two-body spin orbit as well as central components, can provide a satisfactory description of the observed energy levels." The results shown under (ANL) are obtained by a less restricted parametrization.

We see from Fig. 1 that even the spectrum of the nucleus ^{61}Ni cannot as yet be very satisfactorily described by any of the approaches considered so far, and consequently none of these can be confidently used as a starting point for the calculation of the energy levels of the neighboring nuclei. Such an approach has, however, recently been followed[8] for $N=32$ nuclei using the Oak Ridge–Rochester shell-model computer program and involving matrices ranging in size up to 454×454. "A moderate amount of rationalization" had to be applied before terming the agreement between theory and experiment as satisfactory, the disagreement for excitation energies of low-lying levels being on the average about 200 keV. The complexity of the problem with another nucleon would only worsen the agreement.

The experimental level scheme for $N=33$ nuclei is presented in Fig. 2 and reveals little similarity from one case to the other. The already inadequate theories for ^{61}Ni do not evidently promise any better success for ^{59}Fe. We have recently obtained[9] a satisfactory description of the properties of the nucleus ^{57}Fe based on the admixture of Nilsson-model orbitals. Here we discuss the application of the single-particle Nilsson model[10]

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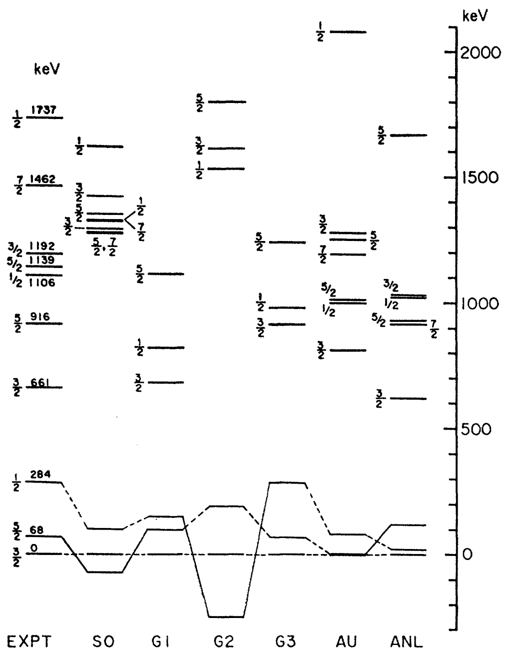

FIG. 1. Low-lying levels in the nucleus ^{61}Ni. The experimental level scheme is taken from Ref. 2. The calculated levels labeled *SO* are for the pairing plus quadrupole-force model (Ref. 4), and those labeled *G1*, *G2*, and *G3* are for the modified Tamm-Dancoff approximation, the BCS method, and the inverse gap equation method, respectively, for the calculation of quasiparticle spectra from Ref. 5. The last two columns labeled AU and ANL are the results of shell-model calculations following the Talmi approach (Ref. 6) and the effective-interaction approach (Ref. 7), respectively. All levels have negative parity.

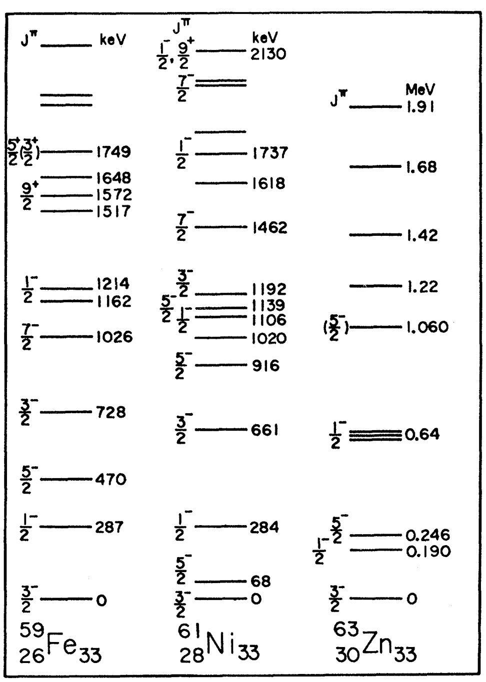

FIG. 2. Experimentally observed spectra of $N=33$ odd mass nuclei.

to describe the observed properties of ^{59}Fe. It may be recalled that the characterization of certain iron isotopes as deformed nuclei was suggested by nuclear-reaction studies[11] several years ago and the rotational-band picture for ^{56}Fe has been discussed[12] following these suggestions.

In the following sections we discuss in the following order—the proposed rotational-band structure with the evaluation of inertial parameters and comparison of these parameters with those obtained for deformed nuclei elsewhere, the determination of the Nilsson-model potential parameters from the lowest states, comparison of other calculated single-particle and rotational states with known experimental data on

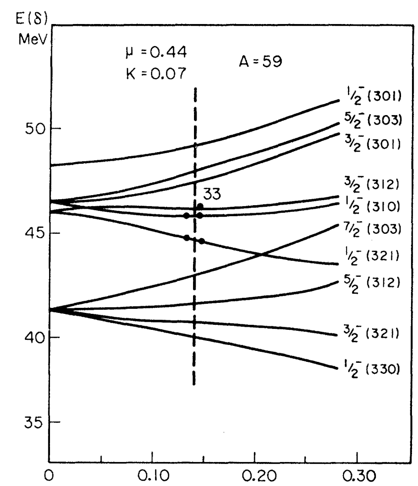

FIG. 3. Nilsson-model energy levels for $N=3$ oscillator shell for $A=59$ with choice of μ and κ as indicated. The broken vertical line indicates the expected deformation region for ^{59}Fe. The dots correspond to the filled neutron orbitals.

excited levels, and a discussion of other observed and unobserved properties for the nucleus ^{59}Fe.

2. ROTATIONAL-BAND STRUCTURE

The eigenvalues for the Nilsson-model Hamiltonian for the oscillator number $N=3$ with the specified values of the parameters μ and κ are plotted in Fig. 3 as a function of the deformation parameter δ. This figure is meant for qualitative guidance in obtaining the expected relative ordering and an order of magnitude estimate of the relative spacing of various single-particle Nilsson orbitals (band heads).

As indicated in the figure, the nucleon number 33 occupies the $\frac{3}{2}^-$ [312] state for any but the smallest deformations, thus unambiguously giving the ground-

[11] C. D. Goodman, J. B. Ball, and C. B. Fulmer, Phys. Rev. **127**, 574 (1962); J. B. Ball, C. B. Fulmer, and C. D. Goodman, *ibid.* **130**, 2342 (1963); D. Beder, Can. J. Phys. **41**, 547 (1963).

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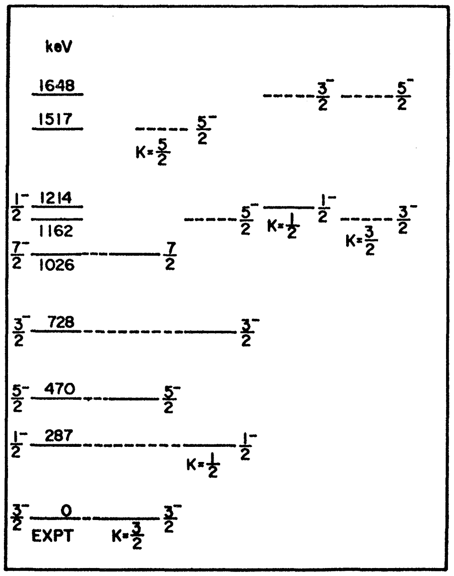

FIG. 4. Proposed rotational-band structure in the observed spectrum of ^{59}Fe. The spin-parity assignments suggested from our study are given on dashed levels.

state spin and parity as $\frac{3}{2}^-$ for these nuclei. This is in contrast to the shell-model picture wherein the 33rd nucleon is in the $f_{5/2}$ orbit on the single-particle model and in order to obtain the ground-state spin of $\frac{3}{2}$ one has to promote a particle from the filled $p_{3/2}$ orbit to the $f_{5/2}$ orbit resulting in the configuration $(p_{3/2})^{-1}(f_{5/2})^2$.

Looking at Fig. 3 we find the first excited state occurring at an excitation energy of 200–300 keV corresponding to a hole in the $\frac{1}{2}^-$ [310] orbit. The observed $\frac{1}{2}^-$ state at 287 keV can thus be identified with the above configuration.

Next, we expect at about the same excitation energy, $\frac{1}{2}^-$ and $\frac{3}{2}^-$ states corresponding to the Nilsson orbitals $\frac{1}{2}^-$ [321] and $\frac{3}{2}^-$ [301]. For deformations in the range of $\delta\approx 0.1$–0.2 they should lie at about 1–2 MeV. The next level corresponding to $\frac{5}{2}^-$ [303] excitation is expected to lie about 400 keV above the $\frac{3}{2}^-$ [301] state. Looking at the experimental spectrum in Fig. 2 we find a $\frac{1}{2}^-$ state at 1214 keV with other states of unidentified spin and parity in the neighborhood.

Following these guidelines we propose the rotational-band structure in the ^{59}Fe spectrum as given in Fig. 4. The ground state $K=\frac{3}{2}$ band is fitted with the formula

$$E_K(I)=E_K{}^0+A[I(I+1)+\delta_{K,1/2}a(-1)^{I+1/2}(I+\tfrac{1}{2})]$$
$$-B[I(I+1)+\delta_{K,1/2}a(-1)^{I+1/2}(I+\tfrac{1}{2})]^2 \quad (1)$$

obtaining the parameters $A=109.2$ keV and $B=1.21$ keV. The nuclear moment of inertia parameter A is comparable to that obtained for the neighboring even-even nucleus ^{58}Fe. As discussed by Mottelson and Nilsson,[13] the physical quantity of interest is

$$\delta\mathcal{I}_{\text{exp}}/\mathcal{I}_{\text{rigid}}=(\mathcal{I}_{\text{odd}}-\mathcal{I}_{\text{even}})/\mathcal{I}_{\text{rigid}}. \quad (2)$$

For evaluation of this quantity we take

$$A_{\text{even}}\equiv\hbar^2/2\mathcal{I}_{\text{even}}\approx\tfrac{1}{6}[E(2^+)],$$
$$A_{\text{odd}}\equiv\hbar^2/2\mathcal{I}_{\text{odd}}\approx\tfrac{1}{5}[E(\tfrac{5}{2}^-)-E(\tfrac{3}{2}^-)], \quad (3)$$

and consider the pairs ^{58}Fe-^{59}Fe and ^{184}W-^{185}W, the latter having the corresponding band structure in the well-established deformed region (the similarity of the spectra of ^{57}Fe and ^{183}W has already been discussed in Ref. 9). The quantity $\delta\mathcal{I}_{\text{exp}}/\mathcal{I}_{\text{rigid}}$ is found to be 12% for the Fe pair and 16% for the W pair.

Next we consider the $K=\frac{1}{2}$ band with observed levels at 287 keV ($\frac{1}{2}^-$) and 728 keV ($\frac{3}{2}^-$). If we assume the same A and B as for the ground band we use Eq. (1) to obtain $a=0.42$. On the other hand let us assume the 1162-keV level to constitute the $\frac{5}{2}^-$ member of the $K=\frac{1}{2}$ band, then setting $B=0$ in Eq. (1) we obtain $A=117$ keV and $a=0.25$. Thus we expect the decoupling parameter to have the value

$$a\approx+0.25\text{–}0.42 \quad (4)$$

Also we have

$$\Delta E=E(\tfrac{1}{2}^-)-E(\tfrac{3}{2}^-)=287\text{ keV}, \quad (5)$$

which according to our picture, is the energy difference between the band heads for the $K=\frac{1}{2}$ and $K=\frac{3}{2}$ rotational bands. It may be noted that in contrast with the level scheme for ^{57}Fe, the two $\frac{3}{2}^-$ levels in ^{59}Fe arising from the $K=\frac{1}{2}$ and the $K=\frac{3}{2}$ bands are widely separated (by 728 keV in ^{59}Fe as compared to 78 keV in unmixed bands in ^{57}Fe) with the result that Coriolis coupling does not bring in any significant band mixing for this nucleus.

3. DETERMINATION OF POTENTIAL PARAMETERS

In Sec. 2 we have evaluated the energy spacing of the lowest two bands and the decoupling parameter for the $K=\frac{1}{2}$ band based on a postulated rotational-band structure for ^{59}Fe. These quantities can be calculated by solving the Nilsson-model[10] Hamiltonian

$$H=H_0{}^{(0)}+\kappa\hbar\omega_0{}^{(0)}R,$$
$$R=\eta U-2l\cdot s-\mu l^2, \quad (6)$$

where $H_0{}^{(0)}$ is the Hamiltonian for a spherically symmetric harmonic oscillator, and U represents the quadrupole distortion. The matrix R is diagonalized for a specified μ to obtain its eigenvalues $r(\eta)$ as a function of the deformation parameter η, and the energy spacings of various single-particle levels are obtained as

$$\Delta E=\kappa\hbar\omega_0{}^{(0)}\Delta r, \quad (7)$$

[13] B. R. Mottelson and S. G. Nilsson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Skrifter. 1, No. 8 (1959).

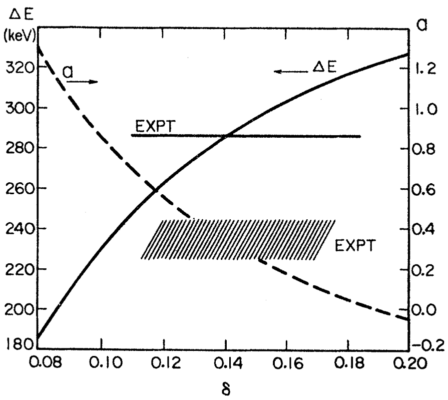

FIG. 5. Plot of the calculated values for the energy spacing ΔE of the $\frac{3}{2}^-$[312] and $\frac{1}{2}^-$[310] single-particle levels (scale on the left) and the decoupling parameter a (scale on the right) as a function of the deformation parameter δ for the choice $\mu=0.44$ and $\kappa=0.07$. The experimental values are also shown in the figure leading to a determination of δ.

with the choice

$$\hbar\omega_0^{(0)}=41A^{-1/3}\text{ MeV}. \quad (8)$$

Instead of η, the κ-dependent deformation parameter δ is employed throughout this study. The eigenfunctions so evaluated also give a value for the decoupling parameter a for the $K=\frac{1}{2}$ bands.

The calculations were carried out for different choices of μ and for a range of κ values as a function of the deformation parameter δ. In view of only two test quantities no unique set of parameters can be defined. Satisfactory fit to ΔE and a could be obtained for choices similar to ones obtained[9] for ^{57}Fe. The results for the choice $\mu=0.44$ and $\kappa=0.07$ are plotted in Fig. 5 in comparison with the "experimental" values for ΔE

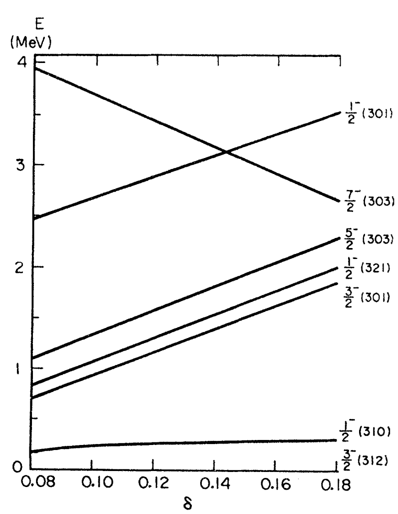

FIG. 6. Calculated excitation energies of various single-particle states relative to the $\frac{3}{2}^-$[312] taken as the ground state for ^{59}Fe.

TABLE I. Potential parameters for the nuclei ^{57}Fe and ^{59}Fe.

Nucleus	μ	κ	δ
^{57}Fe	0.42 to 0.46	0.05 to 0.08	0.16±0.01
^{59}Fe	0.44	0.07	0.14±0.02

and a from Eqs. (4) and (5). It is seen that $\delta\approx(0.14\pm0.02)$ yields satisfactory agreement; the uncertainty quoted corresponds to less than 1% variation in ΔE. The potential parameters for the nuclei ^{57}Fe and ^{59}Fe are quite similar as shown below in Table I.

4. OTHER SINGLE-PARTICLE STATES

A further check on these parameters is provided by other observed single-particle states; alternatively the model can be used to predict these states. The Nilsson-model Hamiltonian was solved for the choice of parameters given above and the excitation energies of other single-particle states were calculated from Eq. (7) for various values of δ. The results for states below 5 MeV are plotted in Fig. 6 for the range of δ values of interest.

The only observed higher single-particle state is $\frac{1}{2}^-$ at 1214 keV which, from Fig. 6, is obtained for $\delta\approx0.12$. If the same value of δ is assumed for other K bands, we may identify 1162 keV as the $K=\frac{3}{2}$ band head and 1517 keV as the $K=\frac{5}{2}$ band head. Then, assuming the same rotational constants as for the lower $K=\frac{3}{2}$ and $K=\frac{1}{2}$ bands, the 1648-keV state corresponds to $\frac{3}{2}^-$ or $\frac{5}{2}^-$ as the second member of the higher $K=\frac{1}{2}$ or $K=\frac{3}{2}$ bands. These assignments are shown in Fig. 4. It will be of great interest if the $\frac{7}{2}^-$ [303], expected to lie in the vicinity of 3 MeV, can be identified, since its spacing relative to all other states decreases with increasing δ.

5. DISCUSSION

At present the only other piece of experimental information available is on the spectroscopic factors derived from ^{58}Fe(d,p) reaction.[1] In the theory of stripping from deformed nuclei[14] the transitions to the rotational states of the same band have spectroscopic factors proportional to the squared coefficients $C_I^2(K)$. Thus for the levels in the ground-state band we have the following results tabulated in Table II.

TABLE II. Spectroscopic factors for the levels in the ground-state band.

I		$\frac{3}{2}$	$\frac{5}{2}$	$\frac{7}{2}$
$C_I^2(K)$	calc	0.20	0.78	0.02
S_j	expt	0.45	0.54	0.08

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The qualitative agreement is quite evident and similar to that obtained for other deformed nuclei. One should not, however, look for a quantitative agreement since the above comparison does not take into account the pairing effect which determines the extent to which a particular single-particle state is filled or empty.

The experimental data on other properties, when available, will certainly be of a great interest in further establishing the validity of the model. According to these calculations the quadrupole moment for the ground state should have a value

$$Q_s=[3K^2-I(I+1)/(I+1)(2I+3)] \times 1.25ZA^{2/3}\delta(1+0.5\delta+\cdots)\times 10^{-26}\ \mathrm{cm}^2 \quad (9)$$
$$=(0.15\pm0.05)\times 10^{-24}\ \mathrm{cm}^2$$

for $\delta=0.14\pm0.02$. Also the band structure proposed in Fig. 4 leads to interband and intraband transition rate estimates which can be easily checked experimentally. For instance, the $E2$ decay of the 1026-keV $\frac{7}{2}^-$ state can either go to 728-keV $\frac{3}{2}^-$ state or to the $\frac{3}{2}^-$ ground state, in one case with $\Delta K=-1$ and in the other case with no change in K, and thus with distinguishable transition rates. Similar selection-rule features will appear in other transition rates and mixing ratios as well. Also it may be noted that both the $K=\frac{1}{2}$ bands are built on hole states whereas the excited $K=\frac{3}{2}$ and $K=\frac{5}{2}$ bands are built on particle states, and such intraband transitions are not favored.

The experimental information on the spin-parity assignments suggested here and on the various electromagnetic moments, transition rates, mixing ratios, etc., will be necessary to assess properly the merits of this approach.

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Excitation Functions for Radioactive Nuclides Produced by Deuteron-Induced Reactions in Iron*

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Cross sections were measured for the production of radioactive nuclides by deuteron-induced reactions in natural iron at bombarding energies below 40 MeV. Deuteron beams of the Oak Ridge isochronous cyclotron were used to bombard stacked iron foils. γ spectra of individual foils were measured with a Ge(Li) spectrometer. Radioactivities with half-lives greater than 20 min were measured. Excitation functions were obtained for ^{55}Co, ^{56}Co, ^{57}Co, ^{58}Co, ^{52}Mn, ^{54}Mn, ^{54}Mn^m, and ^{51}Cr. Cross sections predicted by a compound-nucleus evaporation theory are in reasonable agreement with the experimental results.

INTRODUCTION

Excitation functions for the production of radioactive nuclides by charged-particle-induced reactions are of interest as part of a continuing study of the residual radiation that is produced in the vicinity of particle acceletators.[1–4] Excitation function data can also contribute to an understanding of the reaction mechanisms involved. Only a few excitation functions for production of radioactive nuclides by deuteron induced reactions in iron[5,6] have been reported. The Ge(Li) γ spectrometer,[7–9] with an energy resolution of a few keV, makes the measurements of such excitation functions relatively simple.

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